Challenges in x-ray science

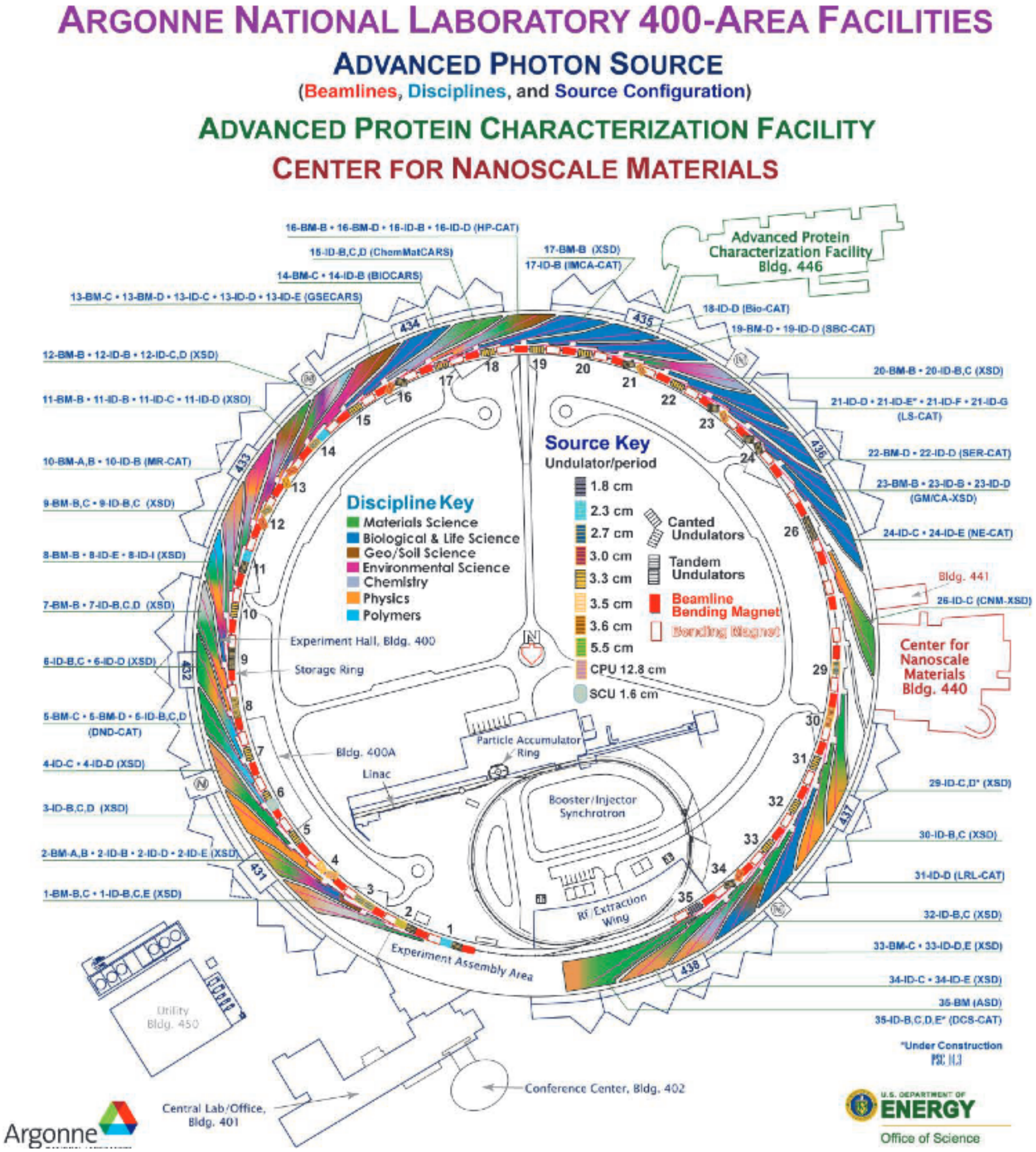
Workshop on Innovative Devices and Systems
Argonne National Laboratory, September 19th 2014

Gabriella Carini

U.S. DEPARTMENT OF ENERGY
Office of Science

SLAC NATIONAL ACCELERATOR LABORATORY

Challenges


ARGONNE NATIONAL LABORATORY 400-AREA FACILITIES
ADVANCED PHOTON SOURCE
(Beamlines, Disciplines, and Source Configuration)
ADVANCED PROTEIN CHARACTERIZATION FACILITY
CENTER FOR NANOSCALE MATERIALS
16-BM-B • 16-BM-D • 16-ID-B • 16-ID-D (HP-CAT)
15-ID-B,C,D (ChemMatCARS)
14-BM-C • 14-ID-B (BIOCARS)
13-BM-C • 13-BM-D • 13-ID-C • 13-ID-D • 13-ID-E (GSECARS)
12-BM-B • 12-ID-B • 12-ID-C,D (XSD)
11-BM-B • 11-ID-B • 11-ID-C • 11-ID-D (XSD)
10-BM-A,B • 10-ID-B (MR-CAT)
9-BM-B,C • 9-ID-B,C (XSD)
8-BM-B • 8-ID-E • 8-ID-I (XSD)
7-BM-B • 7-ID-B,C,D (XSD)
6-ID-B,C • 6-ID-D (XSD)
5-BM-C • 5-BM-D • 5-ID-B,C,D (DND-CAT)
4-ID-C • 4-ID-D (XSD)
3-ID-B,C,D (XSD)
2-BM-A,B • 2-ID-B • 2-ID-D • 2-ID-E (XSD)
1-BM-B,C • 1-ID-B,C,E (XSD)
17-BM-B (XSD)
17-ID-B (IMCA-CAT)
Advanced Protein Characterization Facility Bldg. 446
18-ID-D (Bio-CAT)
19-BM-D • 19-ID-D (SBC-CAT)
20-BM-B • 20-ID-B,C (XSD)
21-ID-D • 21-ID-E* • 21-ID-F • 21-ID-G (LS-CAT)
22-BM-D • 22-ID-D (SER-CAT)
23-BM-B • 23-ID-B • 23-ID-D (GM/CA-XSD)
24-ID-C • 24-ID-E (NE-CAT)
Bldg. 441
26-ID-C (CNM-XSD)
Center for Nanoscale Materials Bldg. 440
29-ID-C,D* (XSD)
30-ID-B,C (XSD)
31-ID-D (LRL-CAT)
32-ID-B,C (XSD)
33-BM-C • 33-ID-D,E (XSD)
34-ID-C • 34-ID-E (XSD)
35-BM (ASD)
35-ID-B,C,D,E* (DCS-CAT)
*Under Construction
PSC 11.3
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Discipline Key
Materials Science
Biological & Life Science
Geo/Soil Science
Environmental Science
Chemistry
Physics
Polymers
Source Key
Undulator/period
1.8 cm
2.3 cm
2.7 cm
3.0 cm
3.3 cm
3.5 cm
3.6 cm
5.5 cm
CPU 12.8 cm
SCU 1.6 cm
Canted Undulators
Tandem Undulators
Beamline Bending Magnet
Bending Magnet
Experiment Hall, Bldg. 400
Storage Ring
Bldg. 400A
Linac
Particle Accumulator Ring
Booster/Injector Synchrotron
RF/Extraction Wing
Experiment Assembly Area
Utility Bldg. 450
Central Lab/Office, Bldg. 401
Conference Center, Bldg. 402
N
Argonne
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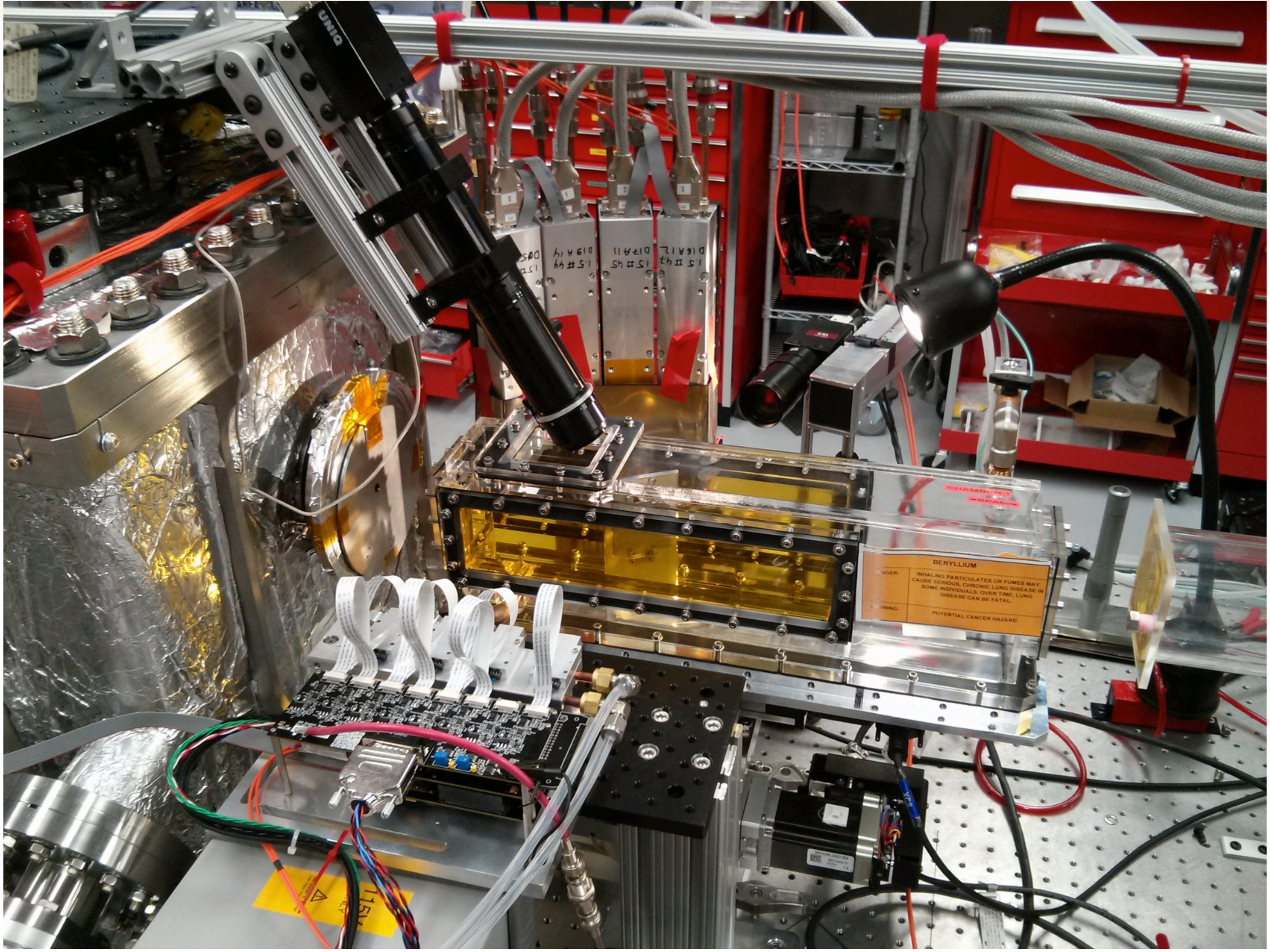
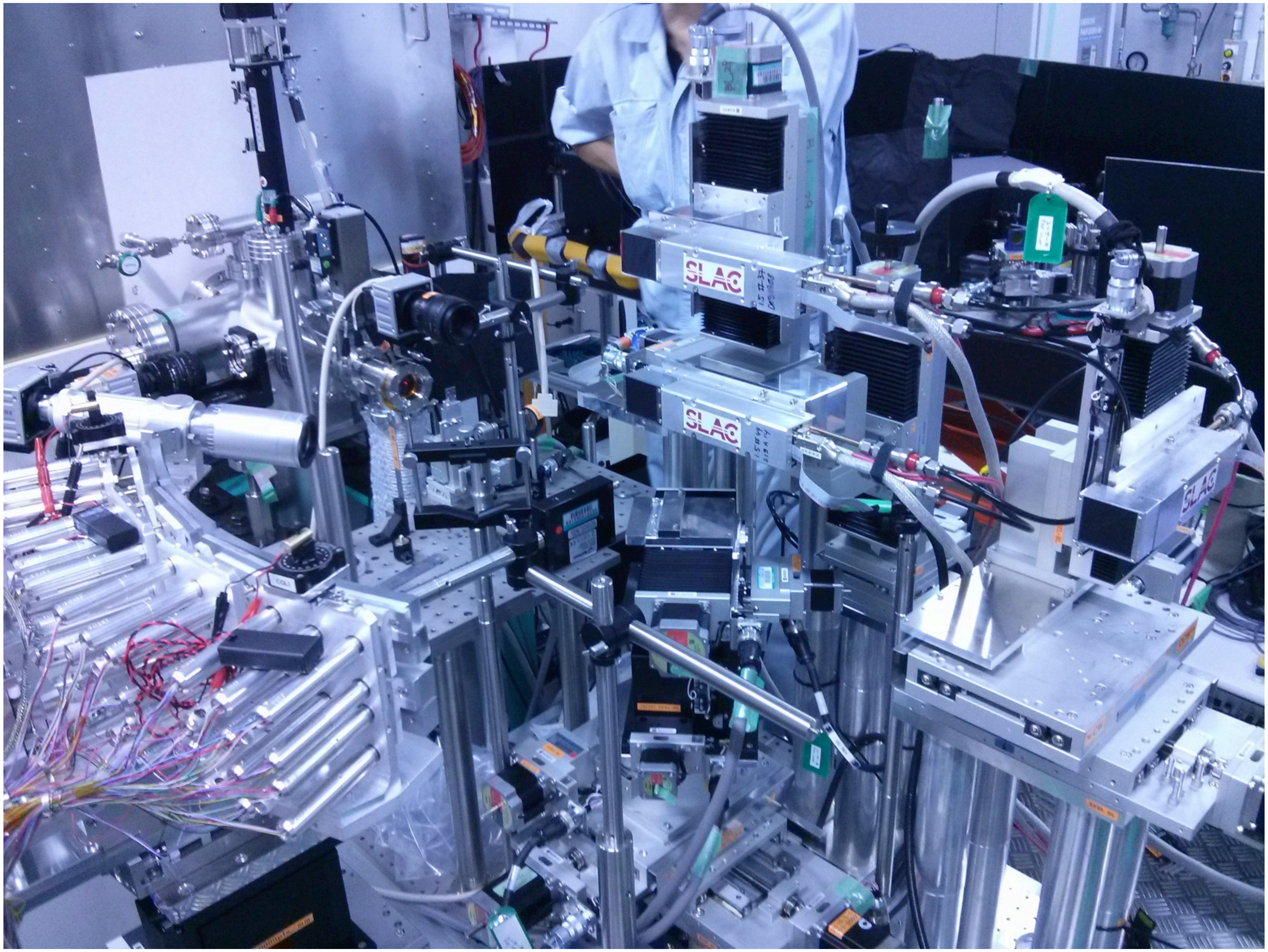
Office of Science

Specific setups for specific experiments



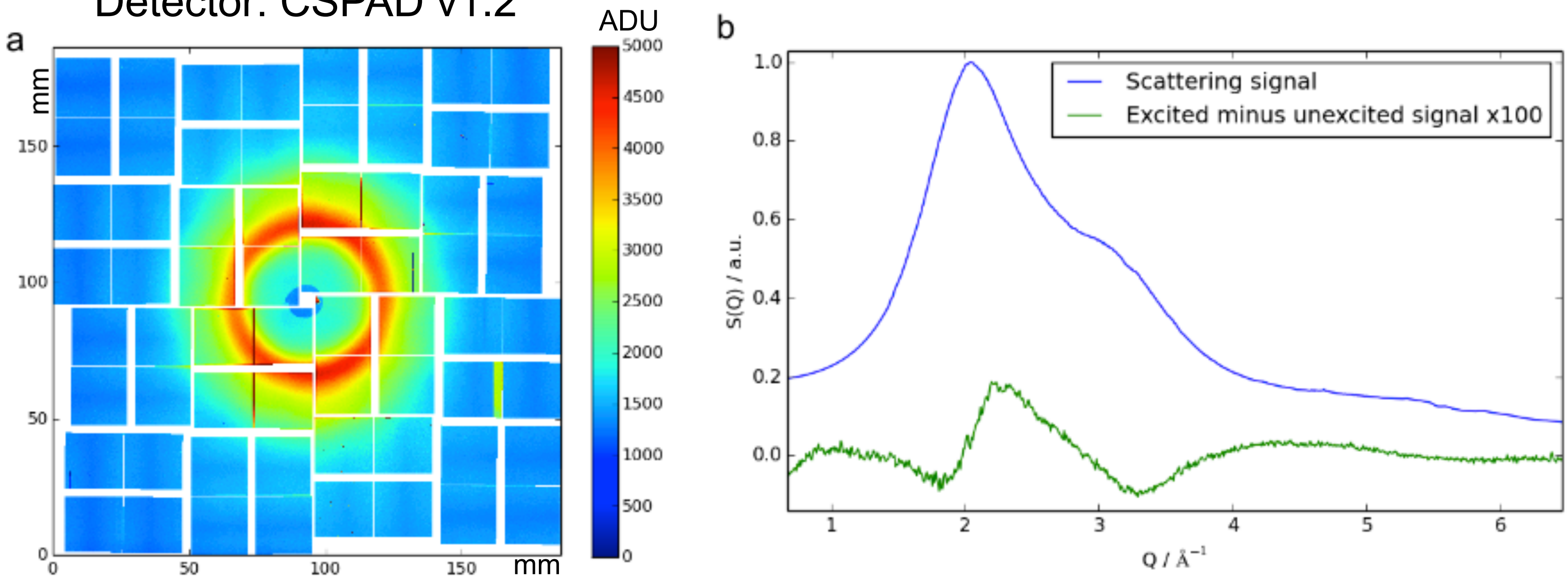
Setups



Typical solution scattering pump probe experiment

Courtesy of Henrik Lemke

Detector: CSPAD v1.2



(a) Diffuse scattering pattern of an aqueous solution (10 images average).
(b) Azimuthally-averaged large dynamic range signal and measured difference signals (170 pulses average).

Challenge:

The large dynamic range signal is changed by ***<<1%*** after excitation with an ultrashort laser pulse.
Inverse transformation of the signal requires ***correct scaling of the small light induced changes throughout the entire intensity range of the scattering pattern (entire range of x-ray pulse fluctuations)***.

Detector needs in x-ray science…

Imaging/scattering:

- Good spatial resolution
- Dynamic range
- Fast and “smart”

Spectroscopy:

- Very high energy-resolution
- High speed

…other common needs

- Efficiency and sensitivity
  - Good entrance window for soft x-rays
  - High stopping power material for hard x-rays
- Fast
  - Detector speed (temporal resolution)
  - Readout speed (frames/second)
- Large solid angle (large area)
  - Scalability
- Radiation tolerant
- Easy to use

Source dependent constraints

FELs

Storage Rings

Continuous source
Information by accumulation

Photons arrive at once
Information per pulse

Zoology

direct conversion (photoeffect)

indirect conversion (scintillation)

energy dispersive

single photon counting

integrating

0D
(point detectors)

1D
(strip detectors)

2D
(imaging detectors)

~~3D
(vertex detectors)~~

Yibin Bai et al, *Teledyne Imaging Sensors: Silicon CMOS imaging technologies for x-ray, UV, visible and near infrared*, SPIE Vol. 7021 (2008)

Photon absorption depth in Silicon

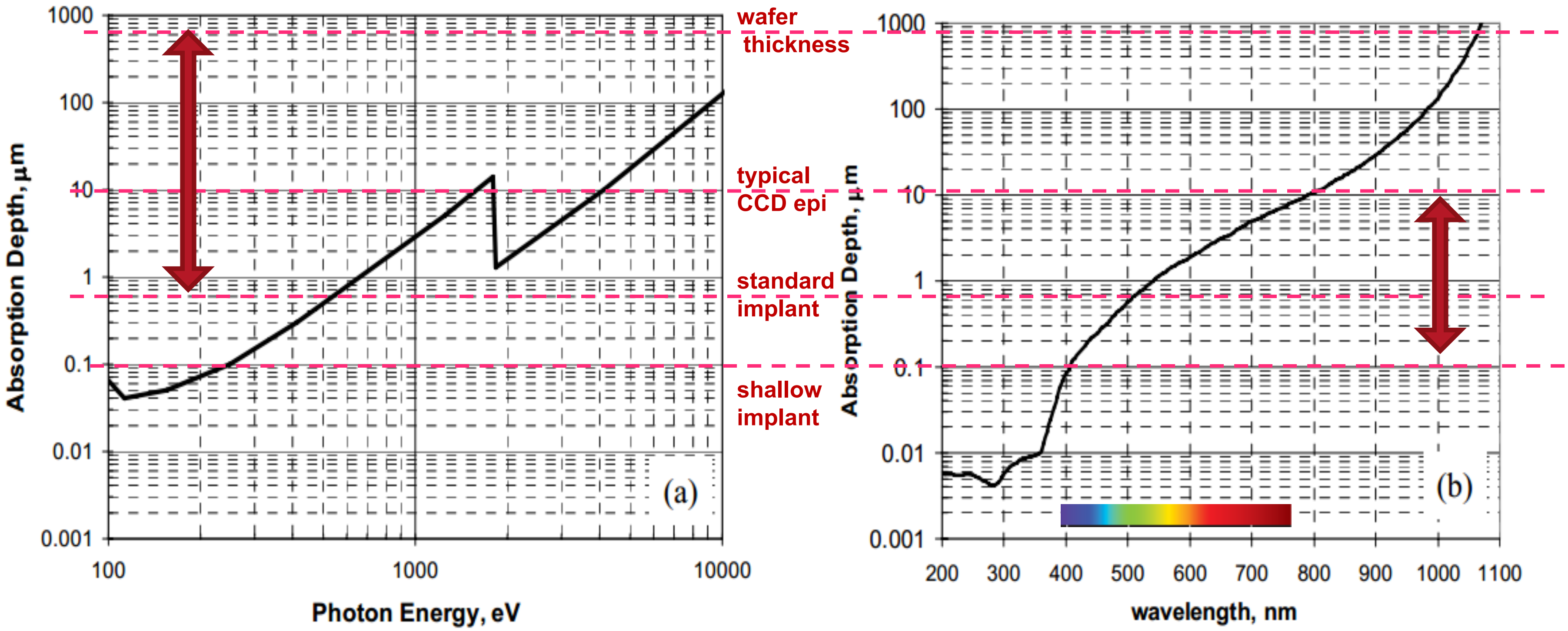


Fig. 7: Absorption depth of photons in silicon as a function of: (a) X-ray energy and, (b) the wavelengths from UV to NIR

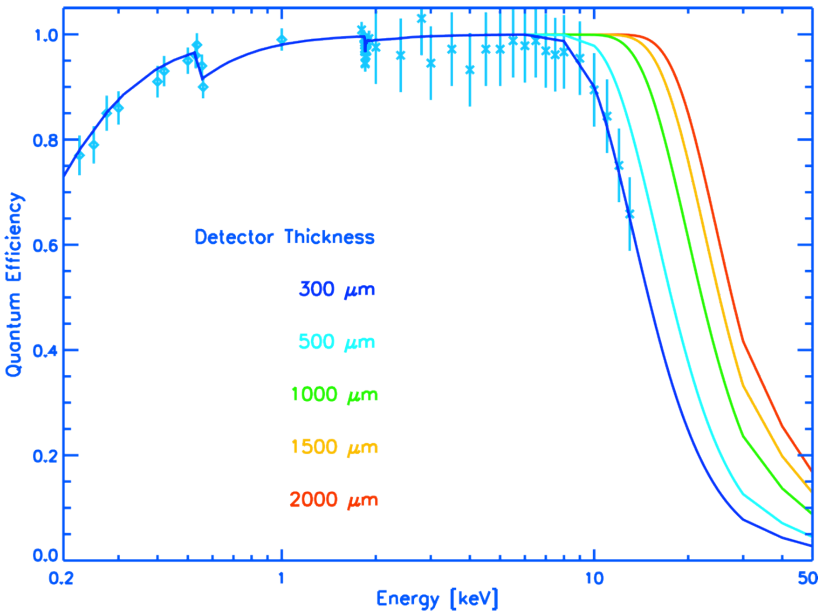
Beer-Lambert law:

I(z) = e (-z/d) ➡

at the absorption depth
63% of the photons are absorbed
-> hard x-ray cameras need tick sensors
37% of the photons are not yet absorbed
-> soft x-ray cameras need thin entrance windows

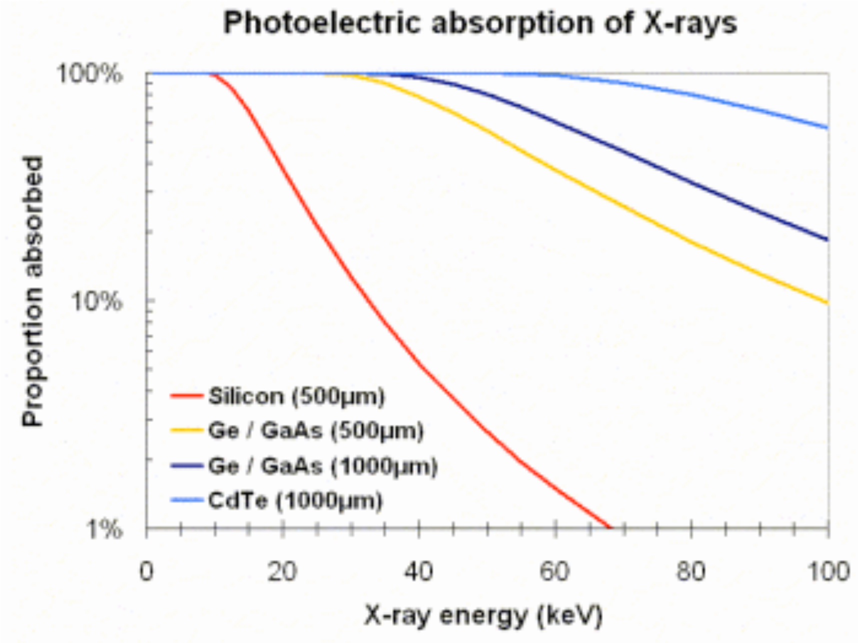
Silicon limitation – other sensor materials

Thicker silicon sensors



From: J. Treis, MPI, Pixel 2008

Other semiconductors for direct detection



http://hasylab.desy.de/instrumentation/detectors/e74464/e106206/index_eng.html

- *Small improvement*
- *High depletion voltage*
- *Parallax*

- *Germanium (‚faster than Si')*
- *GaAs (‚faster than Si')*
- *CdTe, CdZnTe*

Pixel detectors: two approaches

Monolithic

CCD

CMOS imagers

- CMOS Monolithic Active Pixel Sensors (MAPS).
- CMOS Silicon On Insulator (SOI).

Hybrid pixel detectors

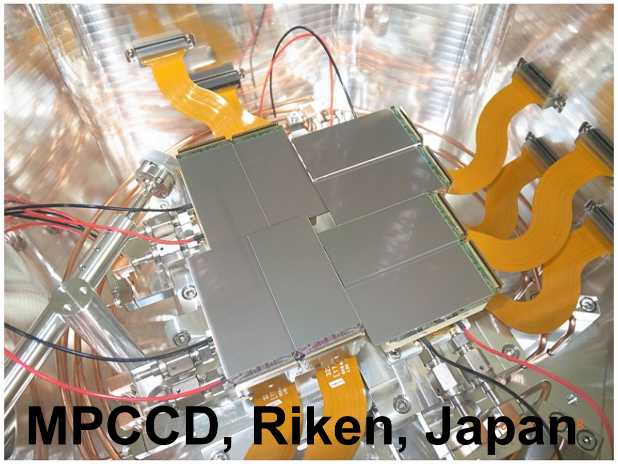
- Sensors in high resistivity silicon (i.e., Pixel Array Detectors (PAD), DEpleted P-channel Field Effect Transistor (DEPFET), Silicon Drift Detectors, X-ray Active Matrix Pixel Sensors (XAMPS)).
- Readout chip in low resistivity silicon - standard IC technology.

…and combination of the above

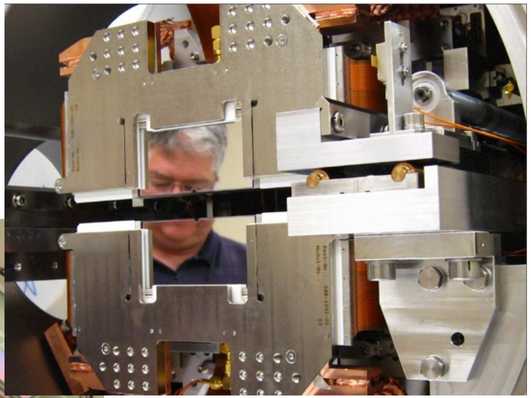
CCDs changed the way we see the world

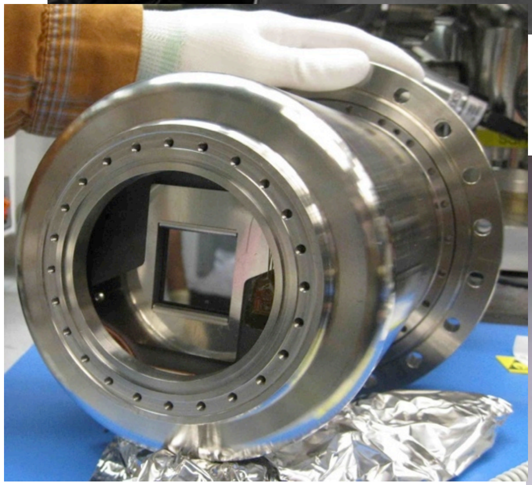
Invention of the CCD in 1969

scintillator fiber coupled to CCD

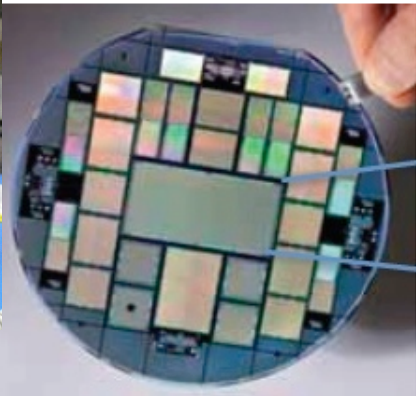


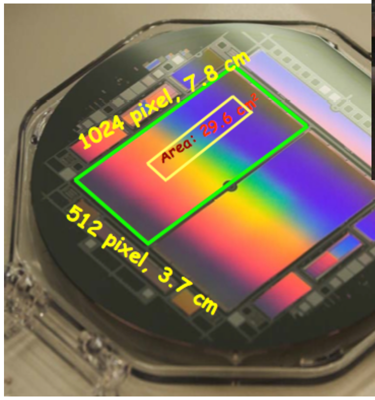
MPCCD, Riken, Japan





FCCD, LBNL





pnCCD, MPG-HLL

CMOS imagers (under development)

SOPHIAS (Riken, Japan)

Fully-Depleted SOI, 5.5-7keV, 30 um x 30 um, 1.92 Mpixel,100 e- (~1 keV), 7 Me$^-$ maximum signal, 60 Hz (multiple gain)

T. Hatsui, International Image Sensor Workshop (IISW), Snowbird, Utah, USA, June 12-16, 2013.

PERCIVAL (RAL, DESY and Elettra)

back-thinned to access its primary energy range of 0.25-1 keV, 25 um x 25 um, 16 Mpixel, single-photon, 1 to ~ 10^5 (500 eV), 120 Hz (gain switching)

http://photon-science.desy.de/research/technical_groups/detectors/projects/percival/index_eng.html

Pixel Array Detectors

It consists of a segmented sensor bonded to a dedicated integrated circuit

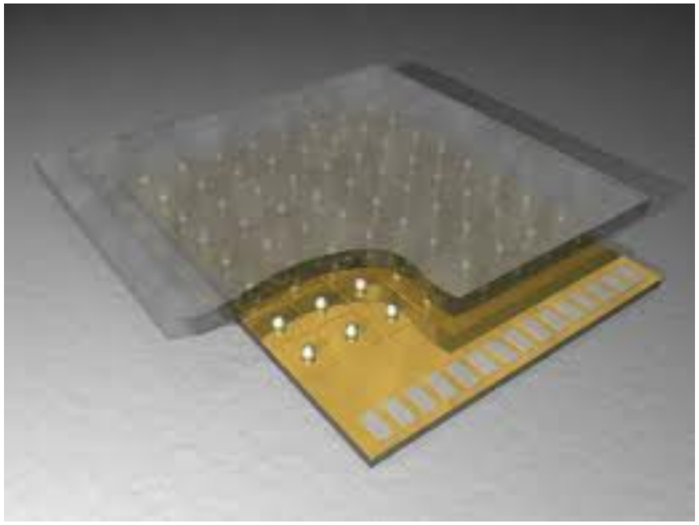


Image from Dectris, LTD

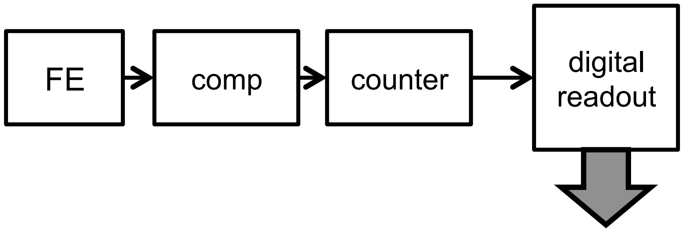
History:

- First developed for High-Energy Physics experiments
  - ATLAS pixel array detector
- Then for applications at synchrotrons:
  - In Europe Detector group at Paul Scherrer Institute
  - In USA Sol Gruner’s group at Cornell University

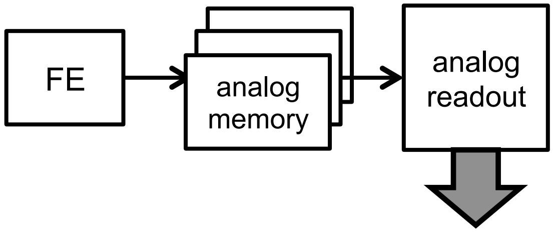
Today many groups are working on that

Application Specific Integrated Circuits

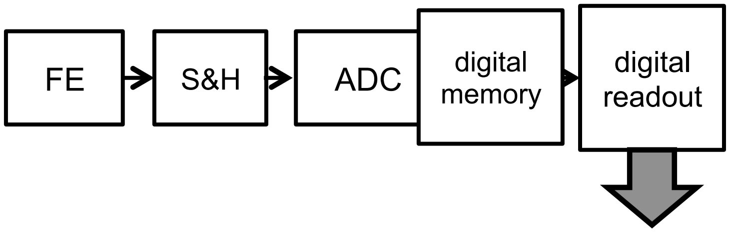
Typical pixel architectures



counting chip



analog integrating – analog readout



analog integrating – digital readout

Good spatial resolution + low noise = better spatial resolution

At single photon rates interpolation may give 1 um position resolution
Spectral information can be available by summing cluster charges

So far scientific CCDs (e.g. pnCCD-MPI/HLL, fCCD -LBNL)

Now low noise integrating pixel array detectors are being developed: ePix 100 (SLAC) and Moench (PSI)

ePix 100

50 um x 50 um pixel, low noise (< 50 e^-) up to 1000 frames / s
Fixed gain - 100 8 keV photon

Synchrotron Radiation News, 27 (4), 14, 2014

MOENCH

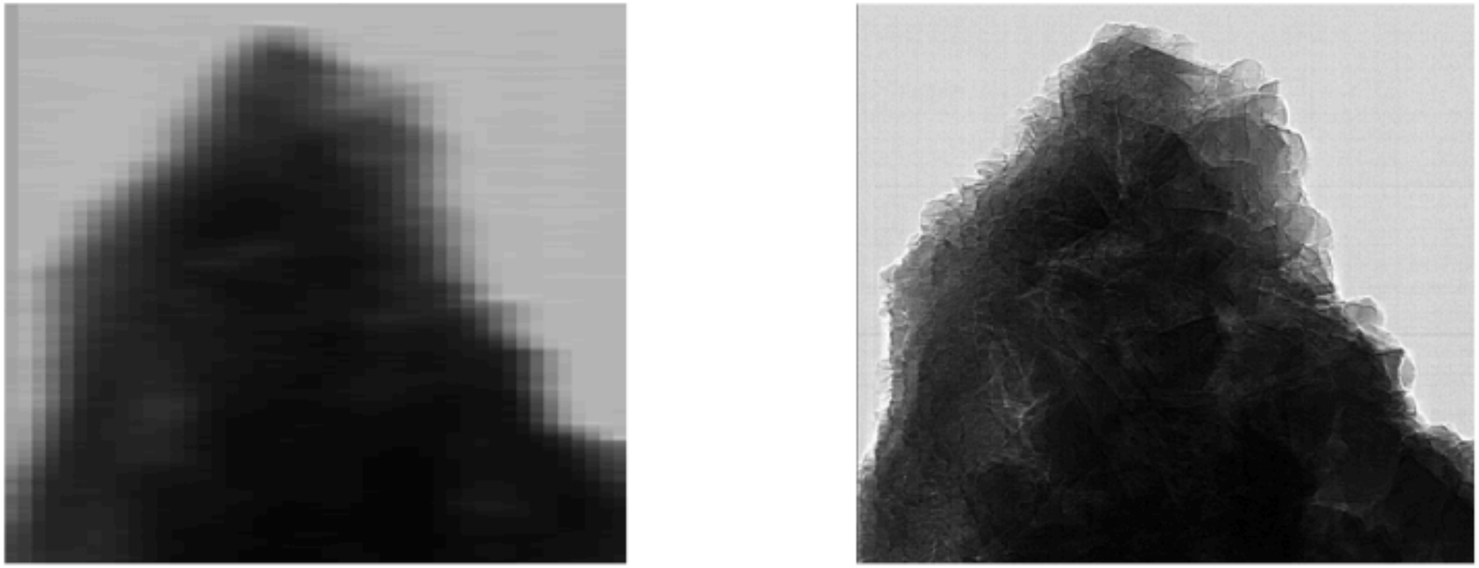
25 um x 25 um pixel, low noise (< 40 e^-)
Different implementation with fixed gain and gain switching - from 15 12 keV photons up to 600 12 keV photons

Synchrotron Radiation News, 27 (4), 3, 2014

Good spatial resolution + low noise = better spatial resolution

At single photon rates interpolation may give 1 um position resolution

Spectral information can be available by summing cluster charges



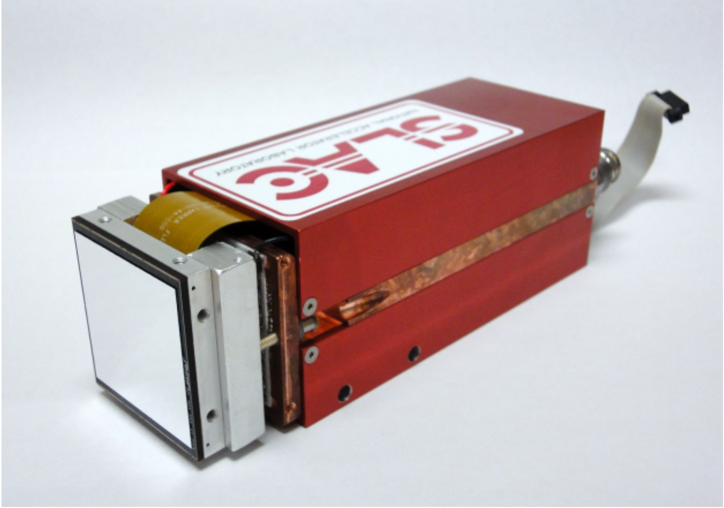
(a)

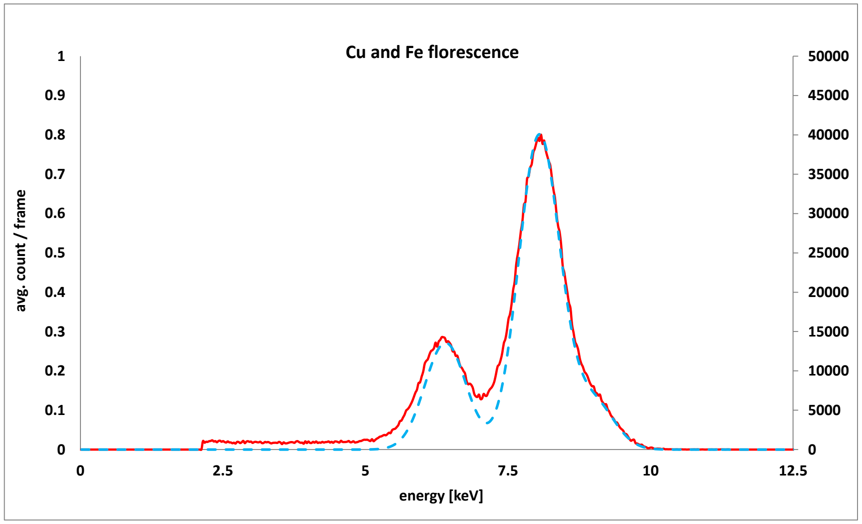
(b)

Figure 4: Image of a kidney stone acquired using GOTTHARD in scanning geometry using a 2 um slit to define the vertical pixel size: (a) analog image acquired with 25 um pitch strips; (b) digital image with 0.5 um virtual pixel obtained after interpolation. Details can be found in [14].

Synchrotron Radiation News, 27 (4), 3, 2014

ePix 100p





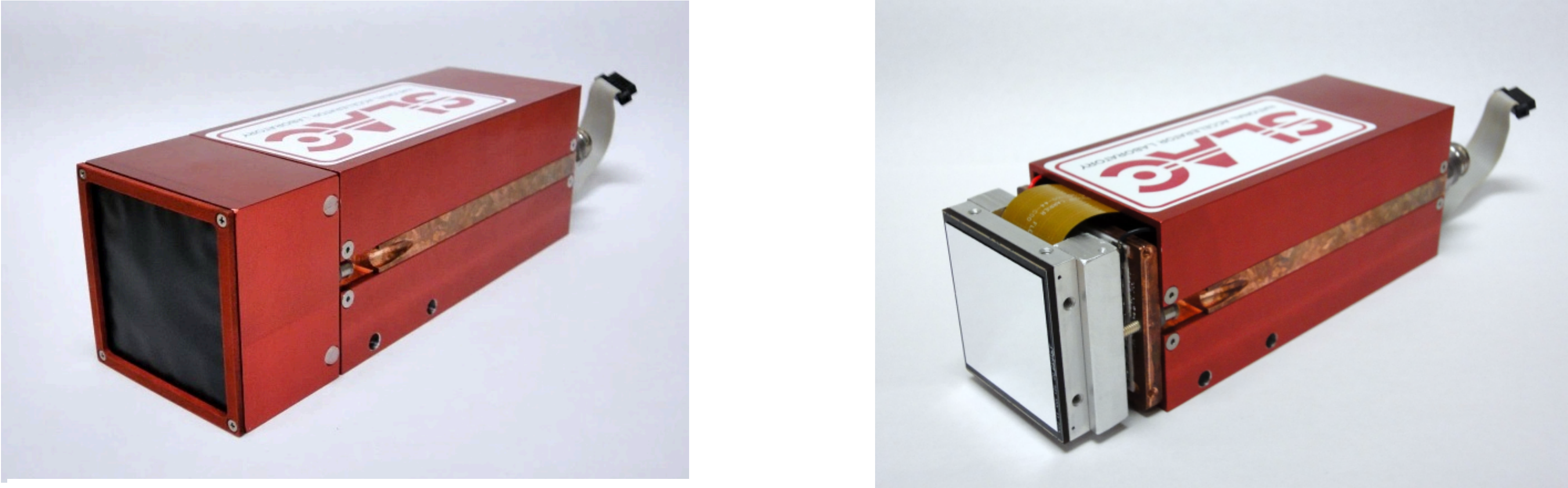
- T= ca -8 C
- Tint = 260 us
- Measured at LCLS

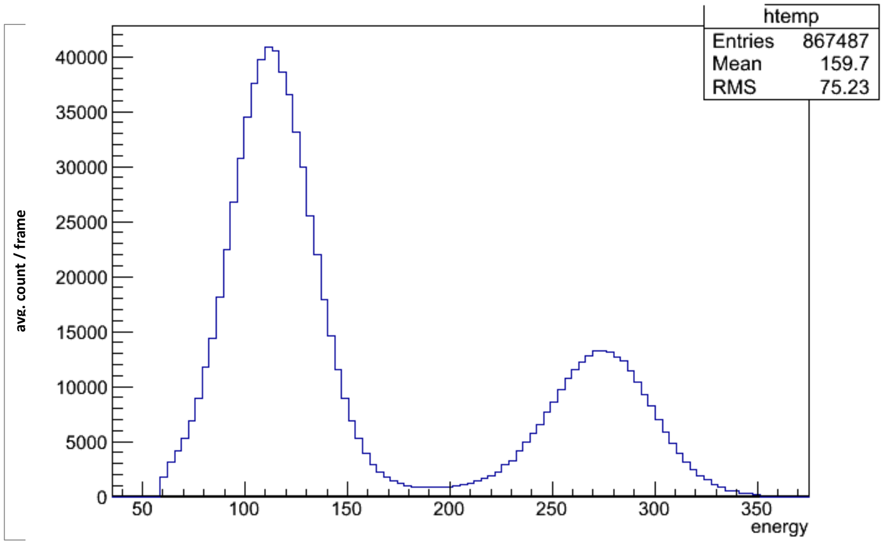
- Cu target and Fe foil
  (Ka: 8.0 keV and 6.4 keV)

- gain corrected

- 0.85 keV FWHM
  -> **99** e- ENC

ePix 100p





SSRL - Ag L line and primary 7.5 keV

- T= ca -8 C
- Tint = 260 us
- Measured at LCLS

- Cu target and Fe foil
  (Ka: 8.0 keV and 6.4 keV)

- gain corrected

- 0.85 keV FWHM
  -> **99** e- ENC

Dynamic range: the gain game?

MMPAD: range extension

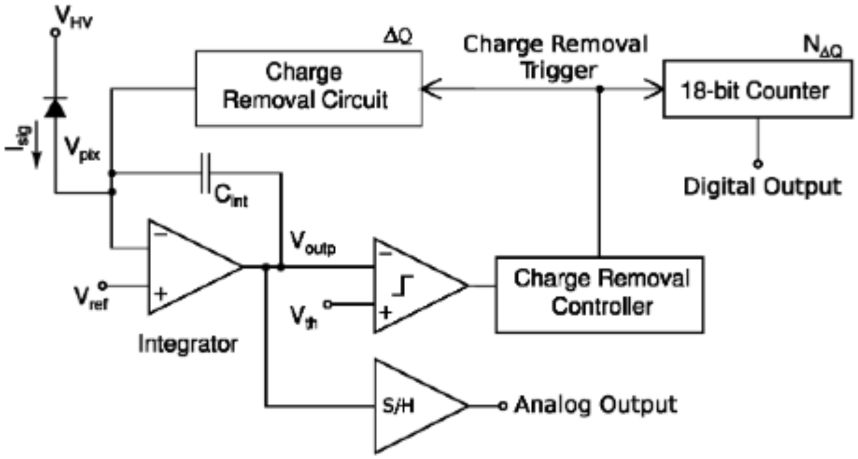
AGIPD, JUNGFRAU, ePix 10k: gain switching

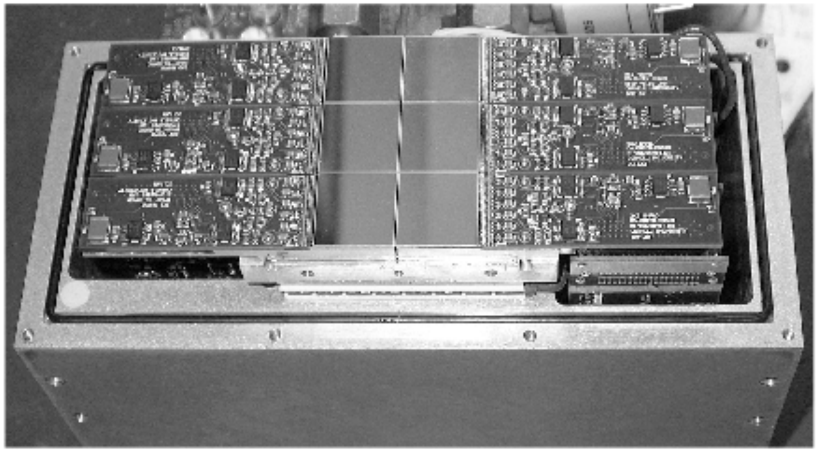
LPD: multiple gains

DSSC: gain compression

Mixed-Mode Pixel Array Detector (MMPAD)

Cornell University and Area Detector System Corporation

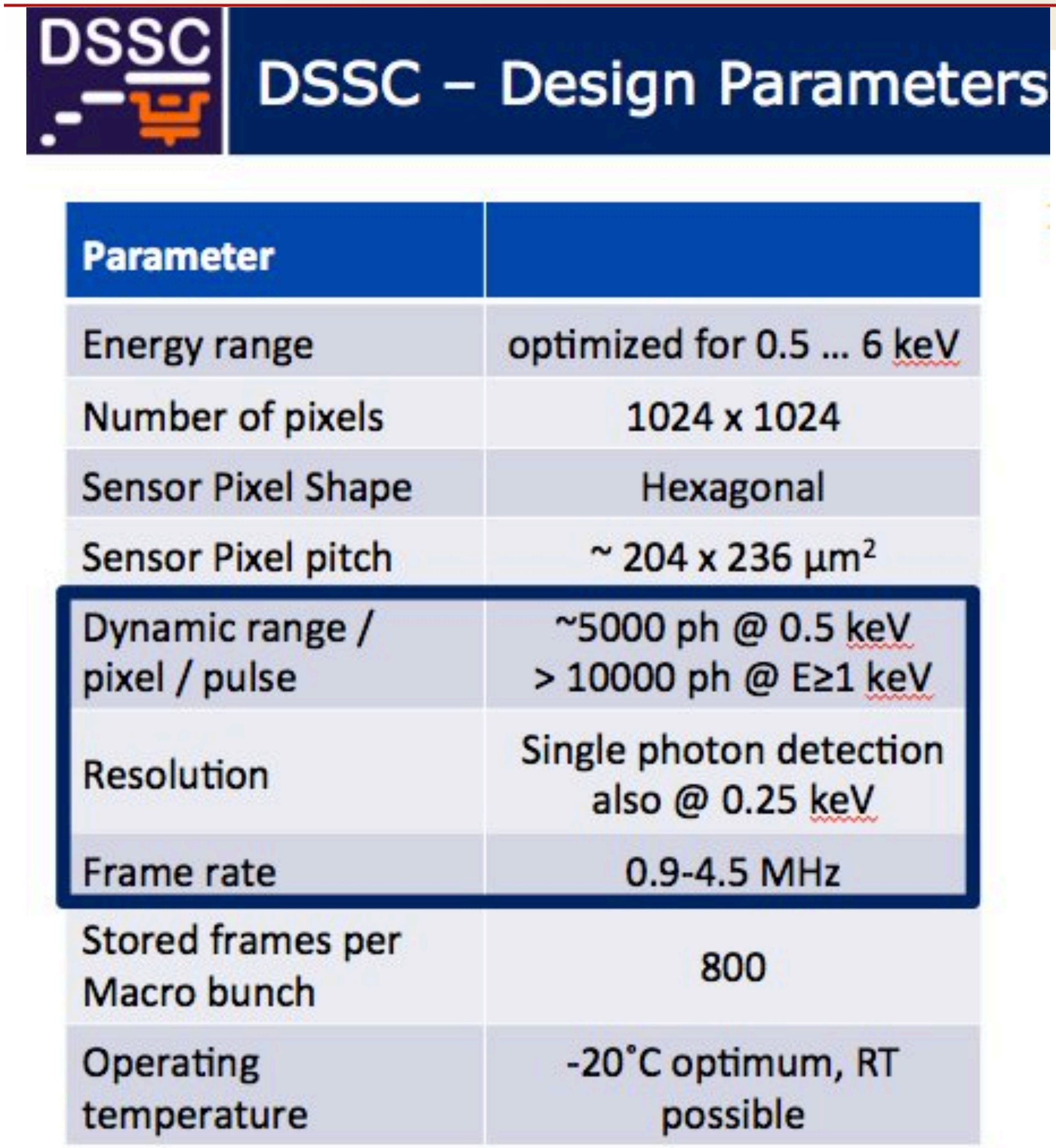




150 um x 150 um, up to 200 photons arriving simultaneously, up to 4.7 10^{7} 8 keV full well, 0. 86 ms read time, > 400 e^- noise, up to 1100 Hz (computer memory) and 200 Hz for continuous storage to disk.

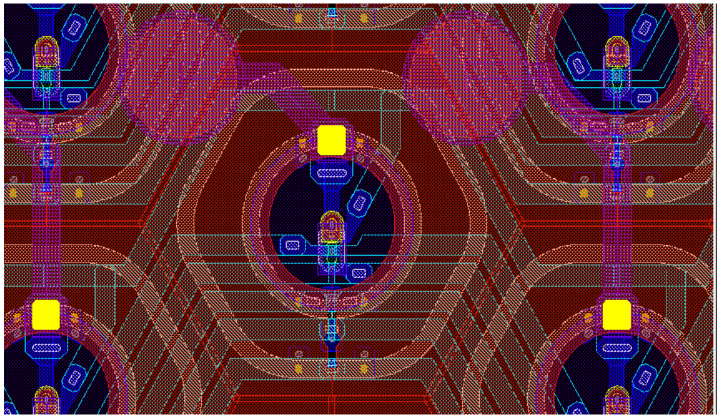
M. Tate *et al.* Journal of Physics: Conference Series **425** (2013) 062004

Gain compression: DSSC

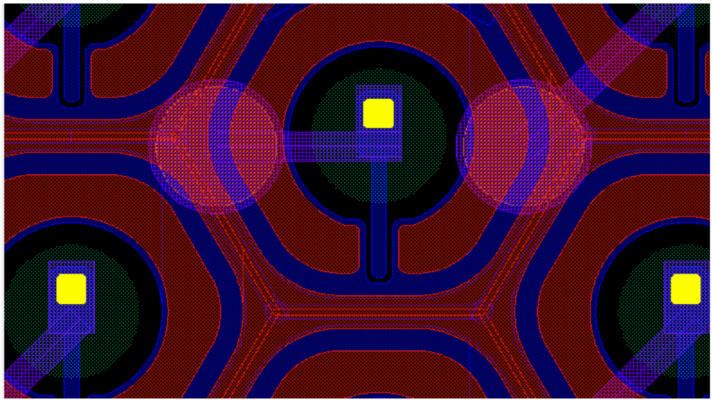


DSSC – Design Parameters

Parameter	
Energy range	optimized for 0.5 ... 6 keV
Number of pixels	1024 x 1024
Sensor Pixel Shape	Hexagonal
Sensor Pixel pitch	~ 204 x 236 µm^2
Dynamic range / pixel / pulse	~5000 ph @ 0.5 keV > 10000 ph @ E≥1 keV
Resolution	Single photon detection also @ 0.25 keV
Frame rate	0.9-4.5 MHz
Stored frames per Macro bunch	800
Operating temperature	-20˚C optimum, RT possible



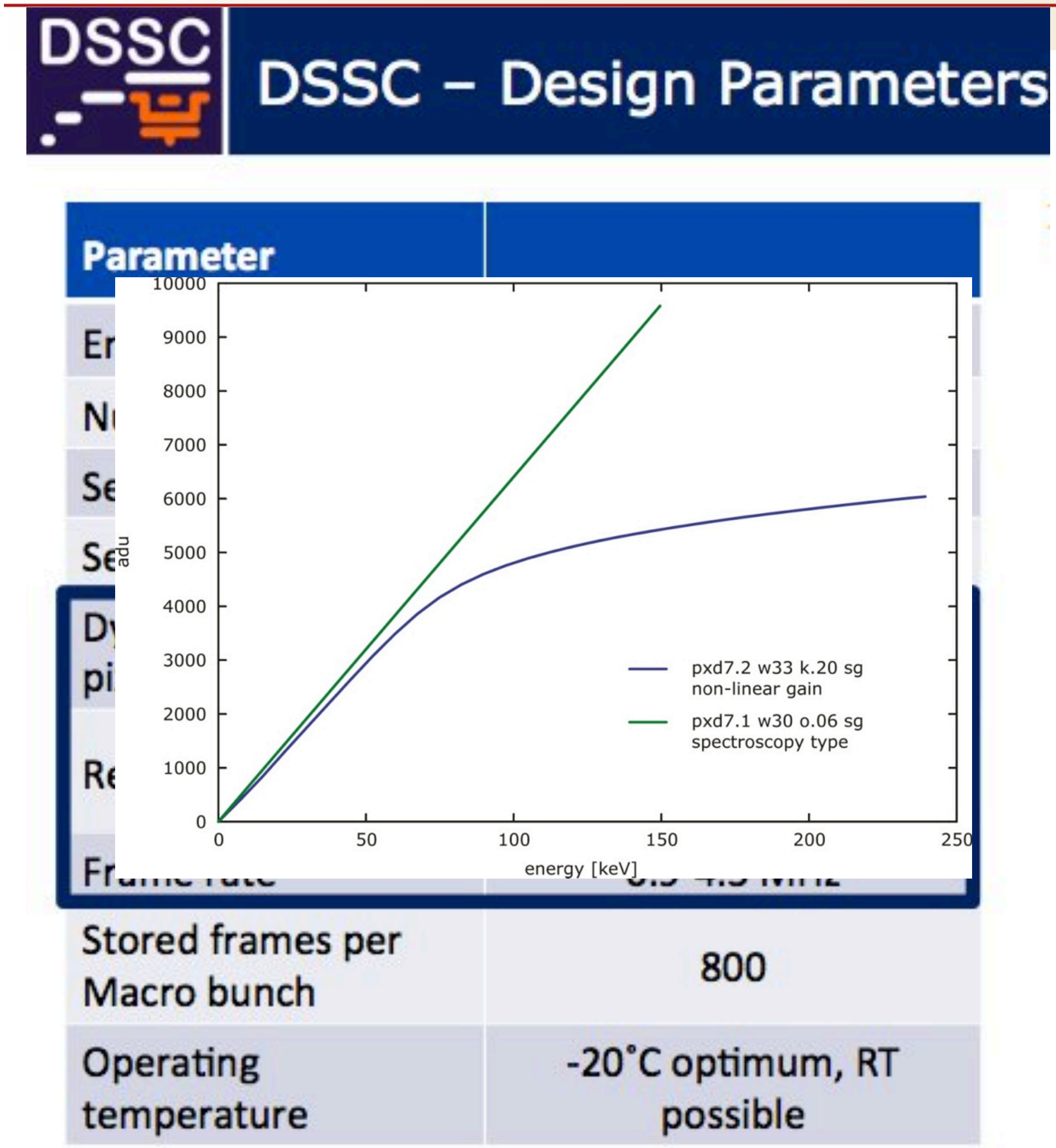
DEPFET (G. Lutz, P. Lechner, PNSensor)
- 2x poly, 2x Al, 1x Cu
- 11 implantations



Mini-SDD (R. Richter, MPG HLL)
- 1x Al, 1x Cu
- 2(3) implantations

Gain compression: DSSC

Matteo Porro
IWORDID14



DSSC – Design Parameters

Parameter	
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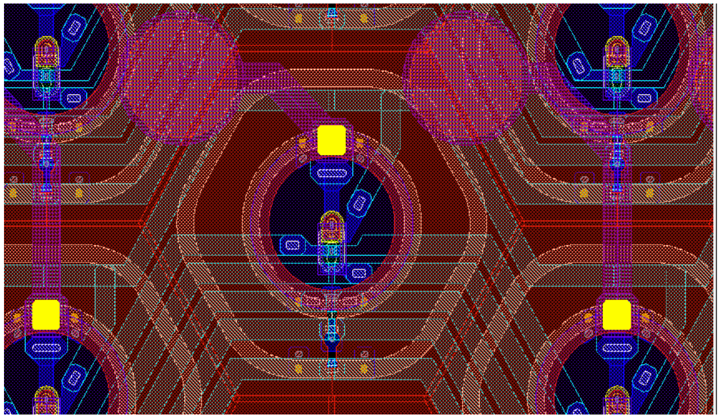
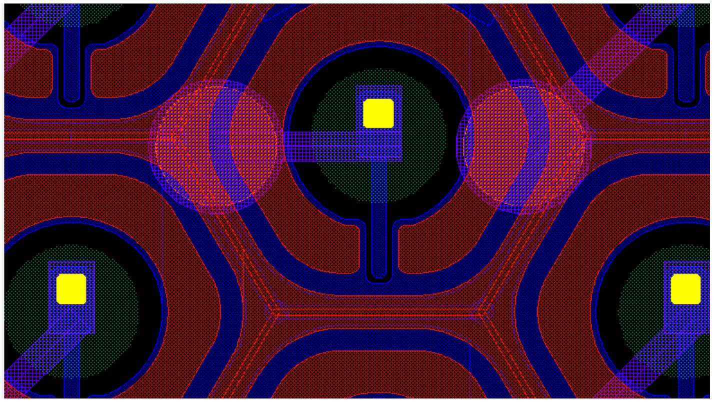
Stored frames per Macro bunch	800
Operating temperature	-20˚C optimum, RT possible



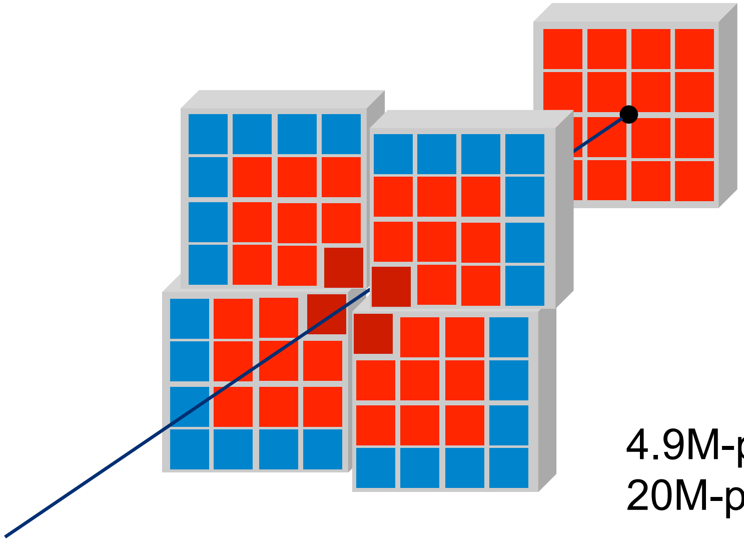
DEPFET (G. Lutz, P. Lechner, PNSensor)
- ➢ 2x poly, 2x Al, 1x Cu
- ➢ 11 implantations



Mini-SDD (R. Richter, MPG HLL)
- ➢ 1x Al, 1x Cu
- ➢ 2(3) implantations

ePix hybrid

ePIX10k module: 135k-pixel
ePIX100 module: 540k-pixel



2.2M-pixel

4.9M-pixel inner ePIX10k region
20M-pixel total (40cm width)

- front detector with fixed (large) hole to simplify cooling and metrology
- could use edge sensitive detectors in the center to minimize dead area
- potential use of a attenuator section in front of back detector
- front and back detector are a single camera, mounted on a single optical bench to simplify alignment and metrology

data rates and link speeds

ePIX one with 0.5Mpixel

- @120Hz 1.0Gbit/sec
- @360Hz 3.1Gbit/sec
- @500Hz 4.3Gbit/sec
- @1kHz 8.7Gbit/sec

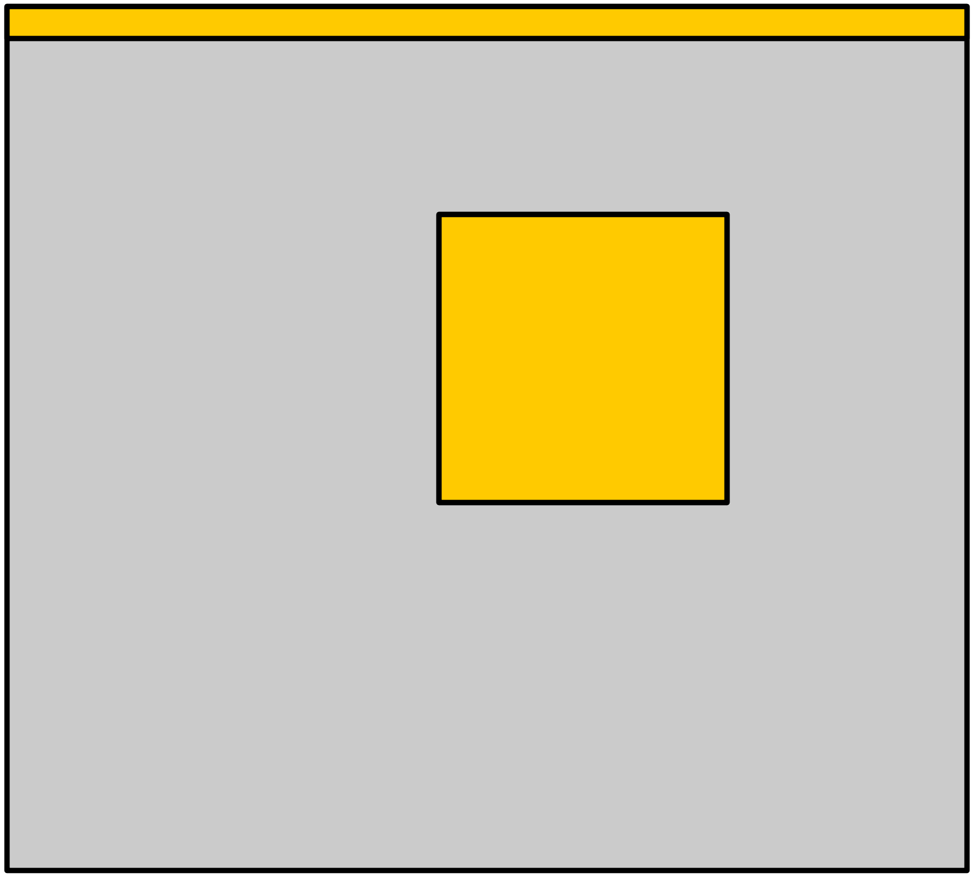
netto data rate for
current PGP link:
2.5Gbit/sec

ePIX four with 2Mpixel

- @120Hz 4.2Gbit/sec
- @360Hz 12.5Gbit/sec
- @500Hz 17.4Gbit/sec
- @1kHz 34.8Gbit/sec

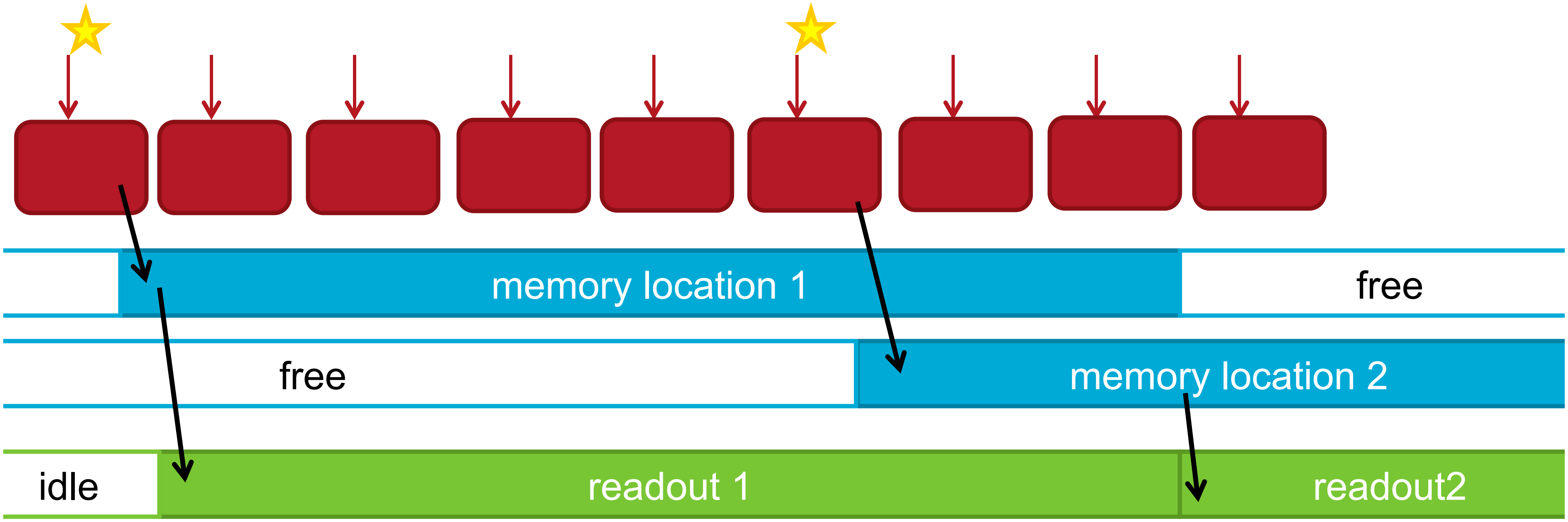
→ Increase link speeds and DAQ capability

ROI, read during capture



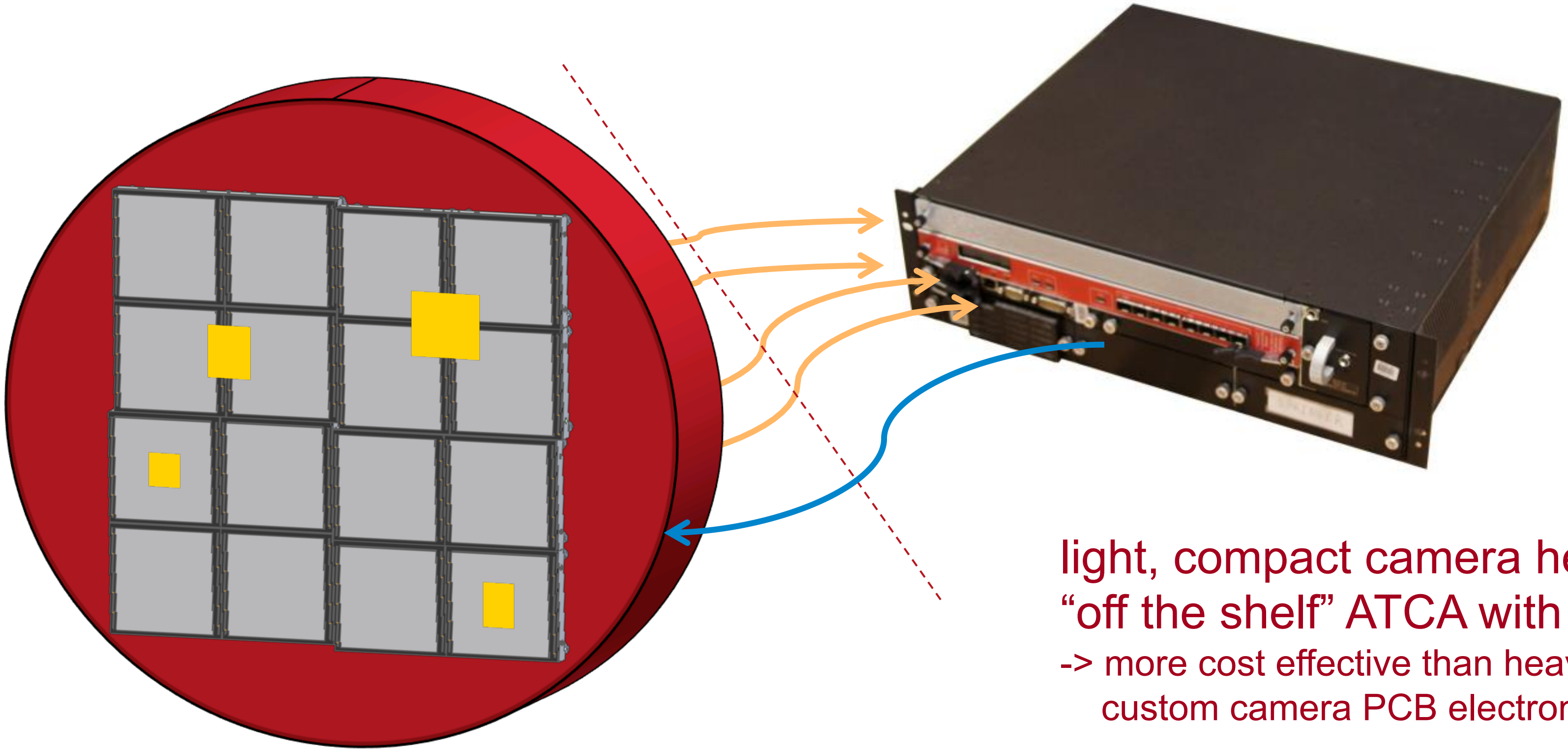
- small region of interest (ROI) is readout at high frame rate
- In every frame of the ROI another small section of the full matrix is readout
- after a number of n frames we collected n ROI frames at high frame rate
- and one full frame at low frame rate
- supporting the acquisition of a slower full frame readout is useful for to observe in “real-time” if alignment or sample properties are drifting.

triggering and read during capture



- In a hybrid pixel detector the (fully parallel) pixel circuitry can operate faster than the ASIC backend (readout) interface
- We could run the front end at higher rates than the backend and readout only selected (triggered) frames

Camera PCB level electronics and DAQ integration



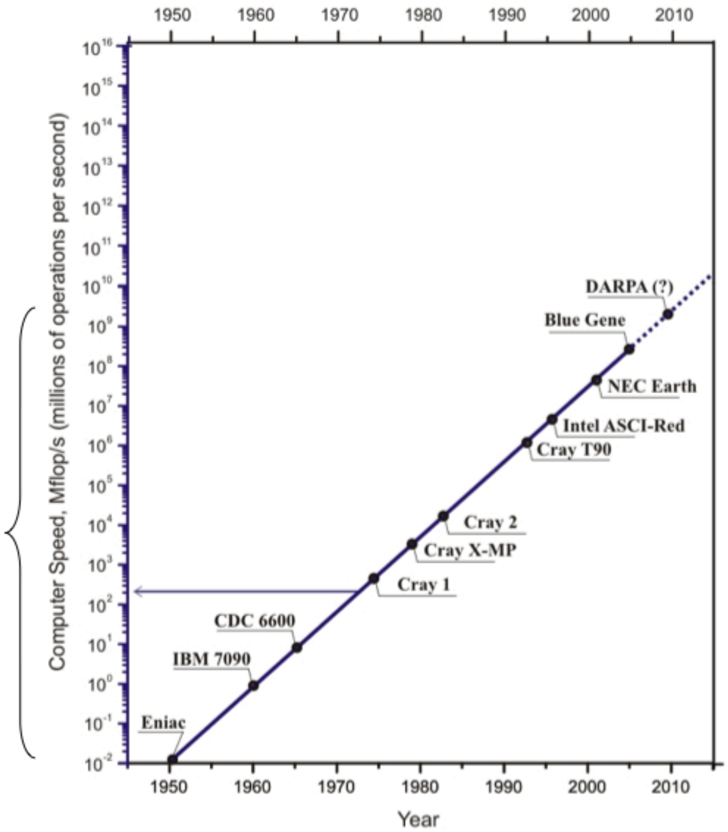
light, compact camera head with "off the shelf" ATCA with RCE

-> more cost effective than heavy custom camera PCB electronics

- To limit the complexity of the cameras PCB level electronics one could aggregate the detector module data and hand it over via next generation high speed serial links to an Advanced Telecommunication Computing Architecture (ATCA) crates and Reconfigurable Computing Elements (RCEs) which can be located up to 20 m away from the camera head.
- The RCE nodes could perform data processing on raw data for the purpose of calibration, online visualization, event selection, binning, averaging and triggering before the final data stream is send to the DAQ system.

Sources/Moore's law

Moore's law for CPU chips

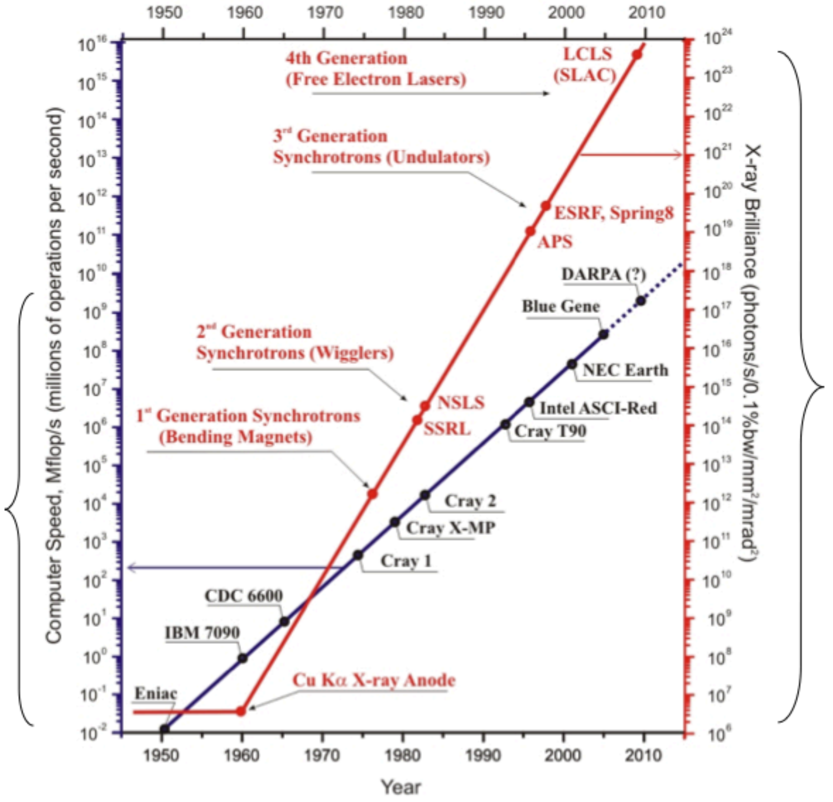


12 orders
of magnitude
In 6 decades

Courtesy of Oleg Shpyrko

Sources/Moore's law

Brilliance is Coherence



12 orders
of magnitude
In 6 decades

18 orders
of magnitude
In 5 decades!

Courtesy of Oleg Shpyrko

Gap with Moore's law? More than Moore and 3D

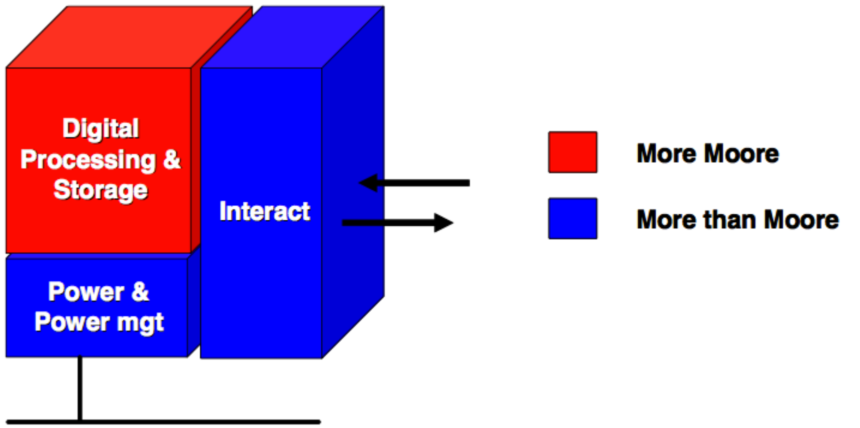
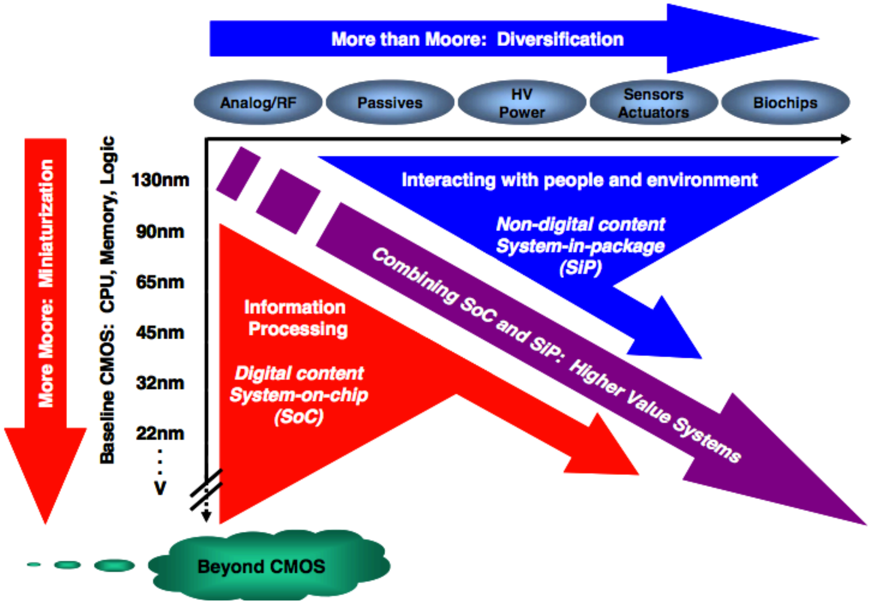


Fig. 4 – "More-than-Moore" devices complement the digital processing and storage elements of an integrated system in allowing the interaction with the outside world and in powering the system.



ital functionalities in an integrated
national Technology Roadmap for
ns ("More Moore") and functional

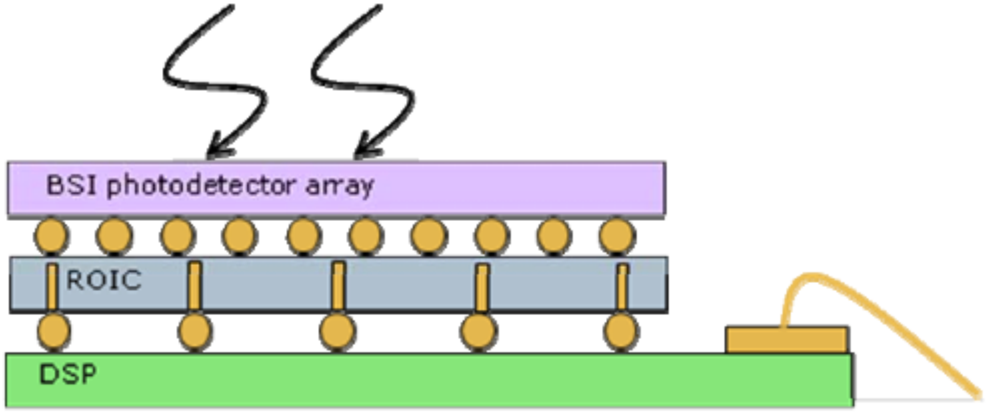
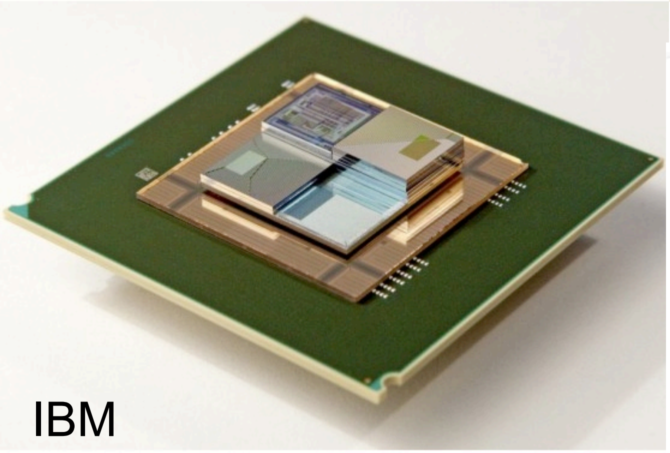


Fig. 5 – 3D integration of a "More-than-Moore" photodetector with "More Moore" read-out and digital signal processing ICs (courtesy of Piet de Moor, IMEC)

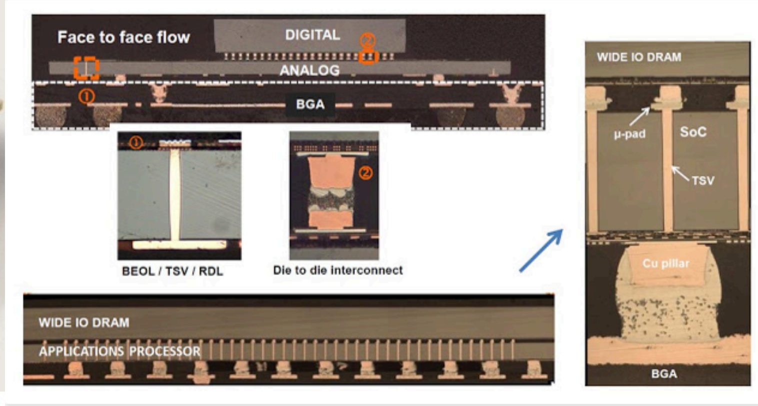
ITRS – More than Moore Whitepaper 2009

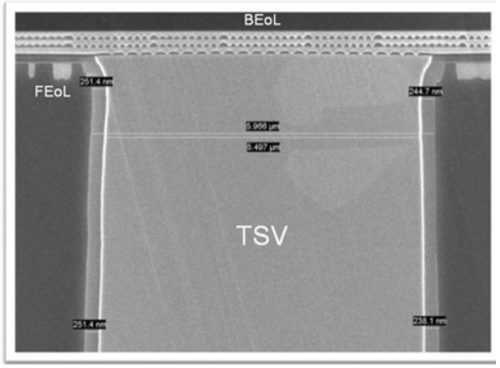
Industry is already implementing 3D (and 2.5D)



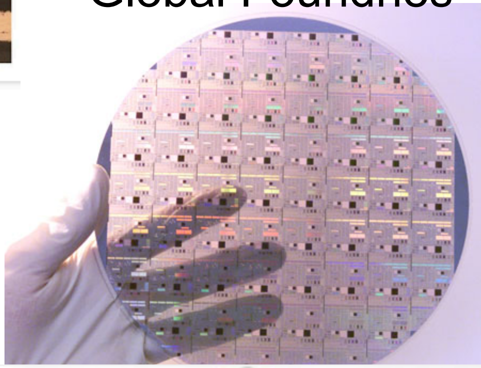
Research 3D chip stack (concept). It is alternate approaches like this, rather than brute-forcing smaller transistors, future of computer.

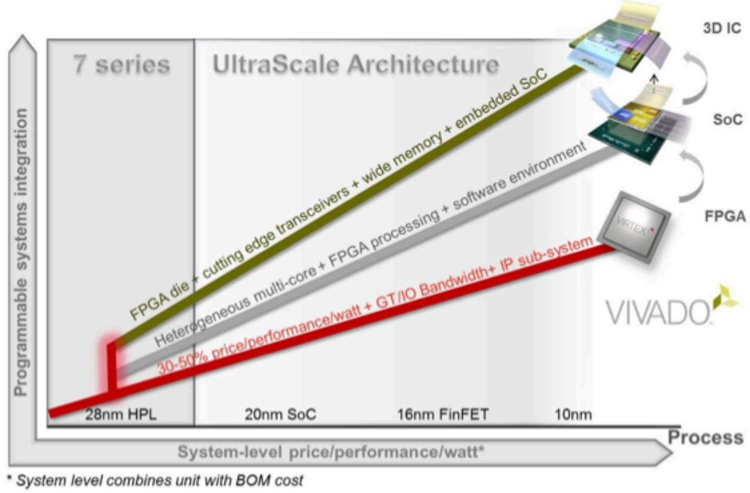
ST microelectronics





Global Foundries



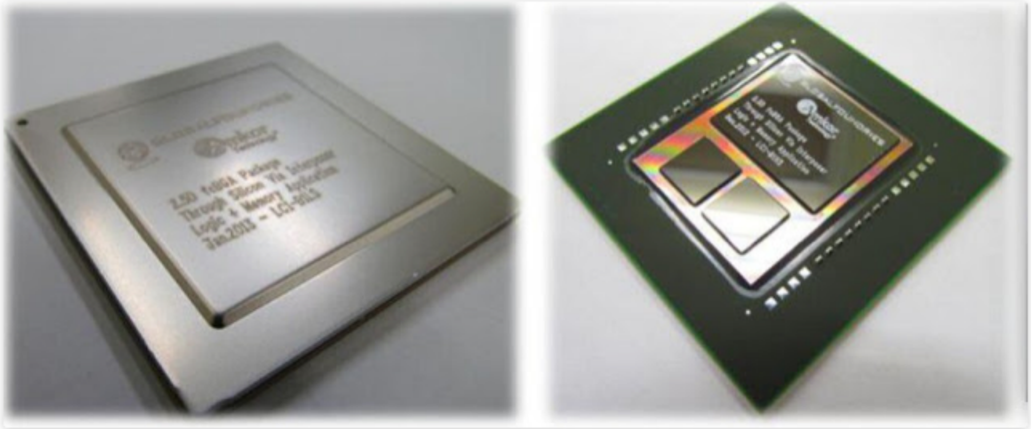


* System level combines unit with BOM cost

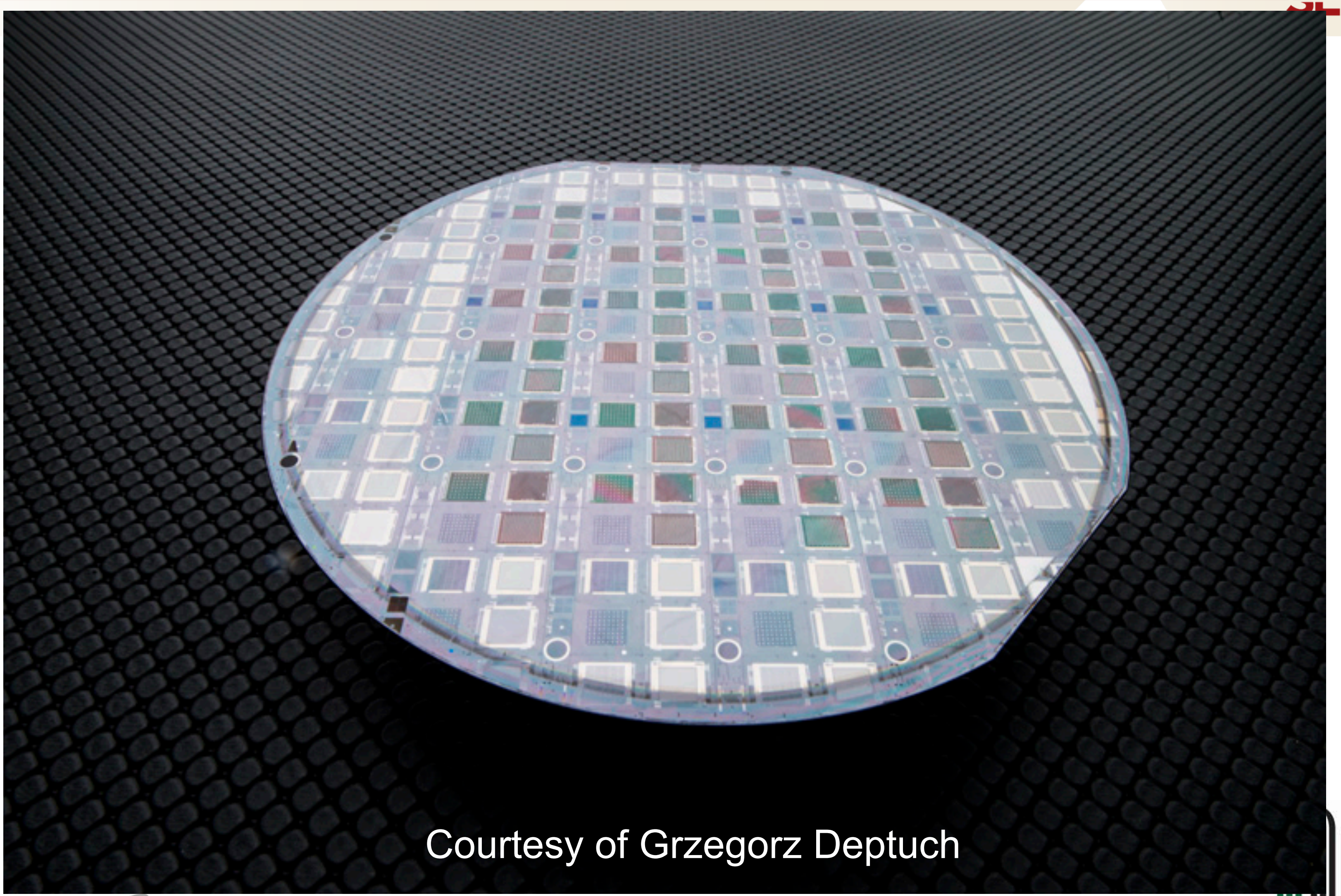
Figure 1: Xilinx continues to expand its leadership in all three areas.

Xilinx

Amkor



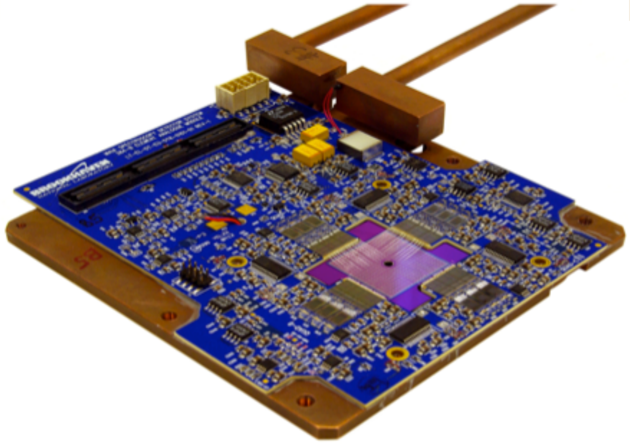
Vertical Integrated Photon Imaging Chip

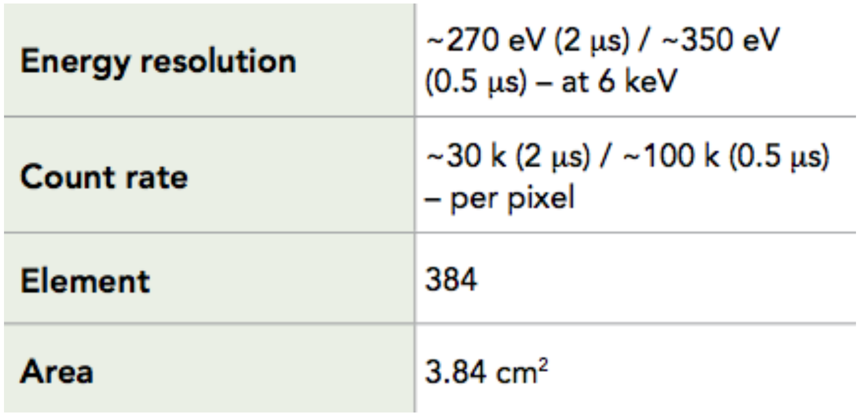


Courtesy of Grzegorz Deptuch

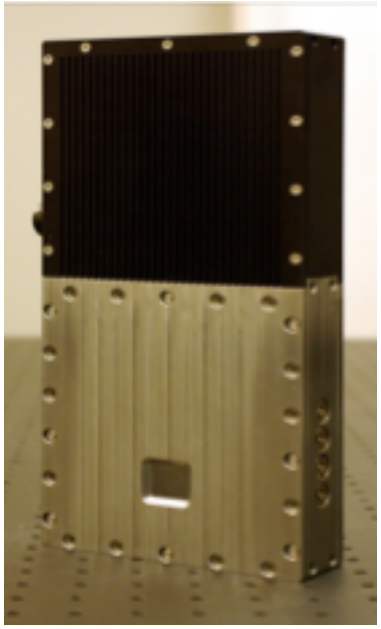
High-speed spectroscopic detectors: Maia (BNL - CSIRO)

P. Siddons, DOE – BES Neutron and X-Ray Detectors Workshop, 2012



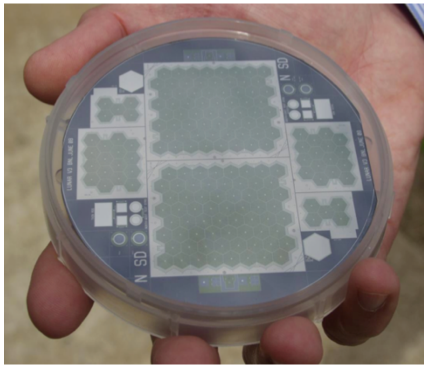


Energy resolution	~270 eV (2 μs) / ~350 eV (0.5 μs) – at 6 keV
Count rate	~30 k (2 μs) / ~100 k (0.5 μs) – per pixel
Element	384
Area	3.84 cm^2



Large solid angle (1.2sr) and real-time processor
Photon event (Peak height, Time-over-Threshold, detector number)
FPGA performs high-speed computation (Dynamic Analysis for deconvolution) and generates elemental maps (photon-by-photon) in real time

Obvious future path with SDDs



Can hybrid pixel array detectors play a role?
HEXID (Hyperspectral Energy-resolving X-ray Imaging Detector, BNL) - Other low noise detectors (e.g. ePix100, Moench)

Rehak *et al.*, Nucl. Inst. Meth. A624 (2010) 260

Courtesy of Kent Irwin

TES x-ray spectrometer collaborators

SLAC / Stanford

Saptarshi Chaudhuri
Hsiao-Mei Cho
Kelly Gaffney
Kent Irwin
Chris Kenney
Dale Li
Michael Minitti
Dennis Nordlund
Tsu-Chien Weng
Christopher Williams

Lund Kemicentrum (Lund, Sweden)

Jens Uhlig

Illinois

Peter Abbamonte
Yizhi Fang

NSLS

Daniel Fischer
Cherno Jaye

NIST

Doug Bennett
Randy Doriese
Dan Swetz
Galen O’Neil
Joel Ullom
Joe Fowler
Carl Reintsema
Gene Hilton
Dan Schmidt

ANL

Antonino Miceli
Tom Cecil
Clarence Chang
Lisa Gades
Tim Madden
Gensheng Wang
Daikang Yan
Jessica McChesney
Fanny Simones
Hongping Yan

Courtesy of Kent Irwin

Sensitivity of TES based X-ray Spectrometers at SSRL (in development)

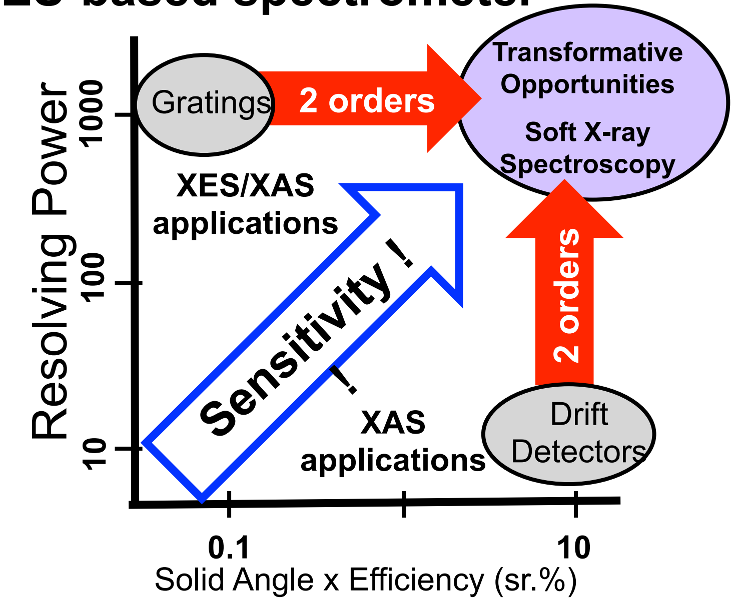
Enabling Ultra-low Concentrations (ppm)

Defects/Dopants	10^{19}-10^{20}/cm^3	=>	10^{17}-10^{18}/cm^3
Surface Sensitivity	1-10% monolayer	=>	0.01-0.1% ML
Solute Sensitivity	10-100 mM	=>	100-1000 uM
Spot Size	10-100um	=>	1-10mm

New Science Opportunities in Material Science, Chemistry, and Biology

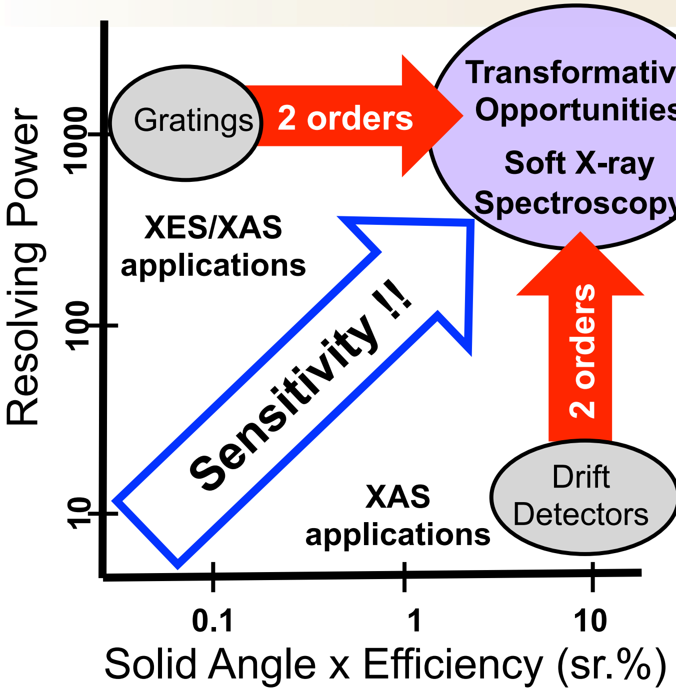
Grating Spectrometer

TES-based spectrometer



Courtesy of Kent Irwin

LDRD-funded TES Spectrometer for SSRL



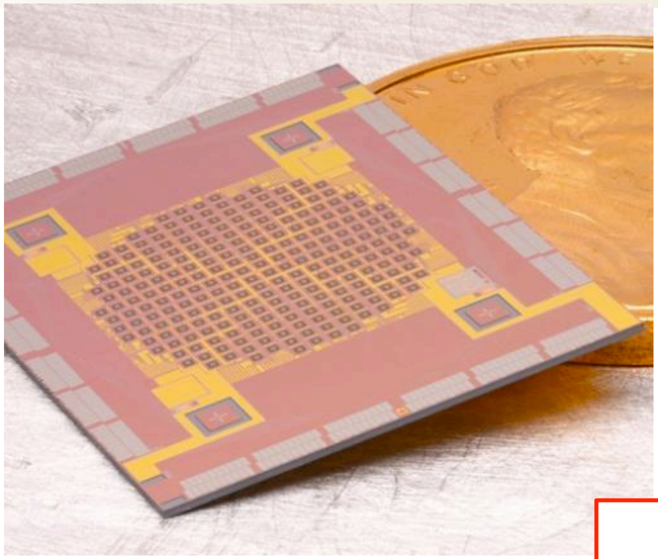
- 240 pixel array

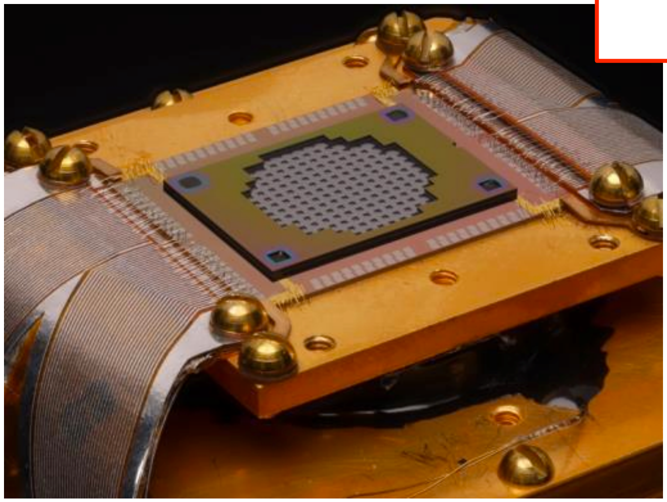
	TES Spectrometer	Grating Spectrometer
Solid Angle	**0.02 sr**	0.0013 sr
Photon Detection Efficiency	**33% N *K*, 58% O *K*, 90% Cu *L*** (dominated by x-ray windows)	<5%
Measurement Energy Range	**250-1000 eV (multiple edges simultaneously)**	~100 eV (single edge, time consuming alignment)
X-ray Beam Focus	None Required	Tight Focus (~few um)
Energy Resolution	1 eV	0.7 eV typical*

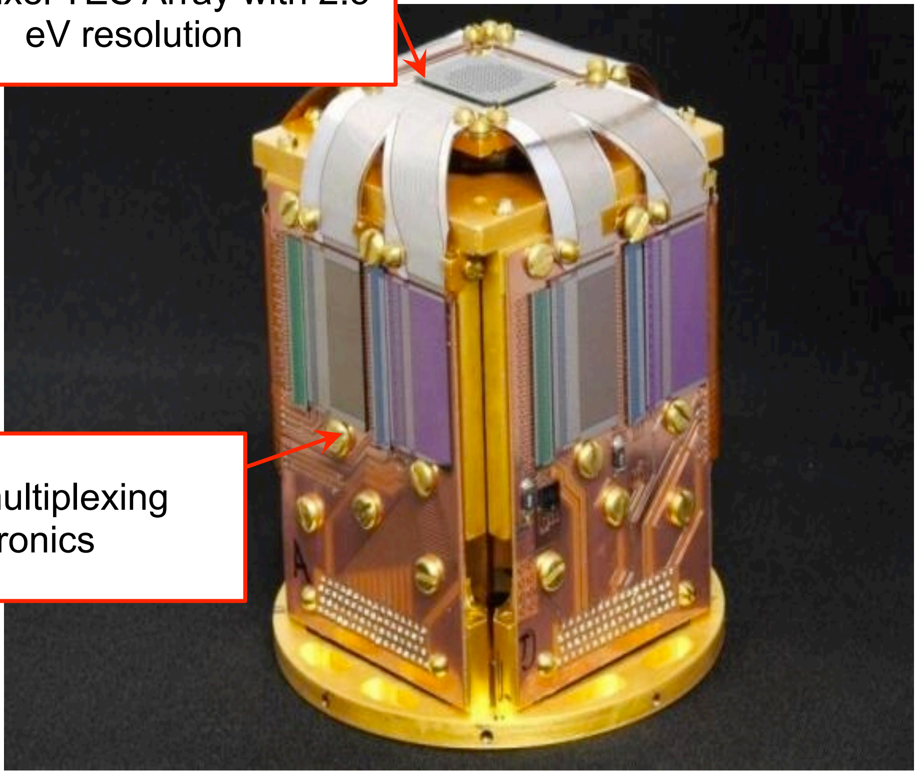
*Can be significantly better, but with much lower efficiency and smaller solid angle

Courtesy of Kent Irwin

TES Spectrometer Arrays







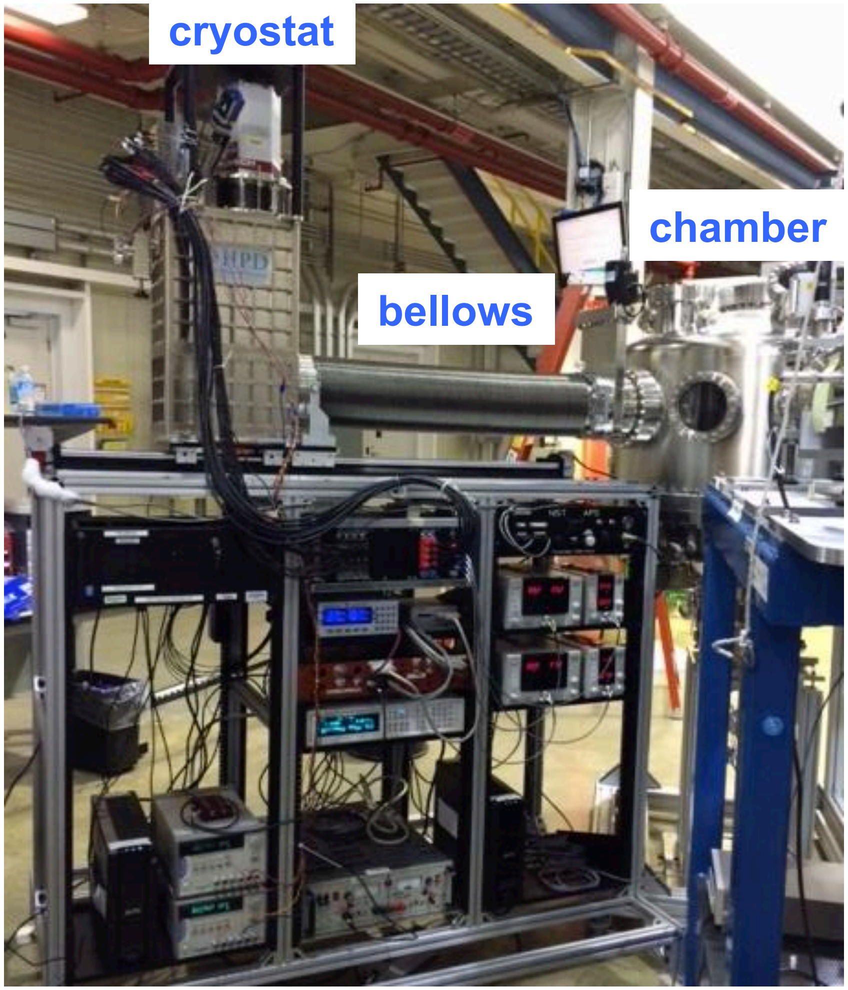
160 Pixel TES Array with 2.5 eV resolution

SQUID multiplexing electronics

We are now deploying a 240-pixel soft x-ray spectrometer array on SSRL BL-10-1

Courtesy of Kent Irwin

Beamline hardware



NSLS U7A beamline

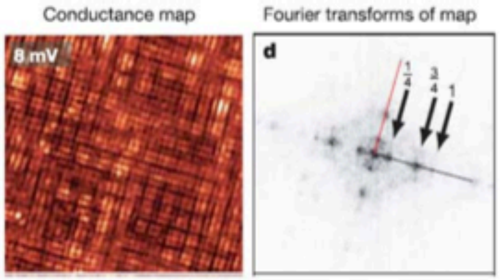
- 200-1400 eV
- Prototype installed Dec., 2011

APS 29ID IEX beamline

- 400-2500 eV
- Installed August, 2014

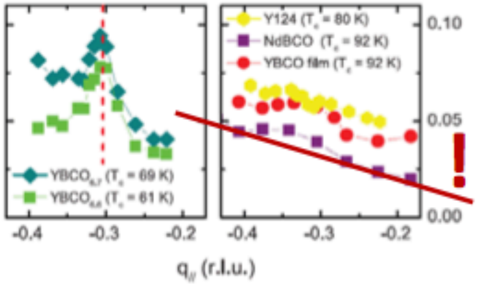
Studying charge order in superconductors using transition edge sensor (TES) detectors, **P. Abbamonte (UIUC), D. Swetz (NIST), et al.**

Short-ranged, glassy charge order – *how pervasive is it*?



There is circumstantial but widespread evidence that local charge order is pervasive in unconventional superconductors, such as copper-oxides and iron-arsenides, and therefore may be integrally related to the mechanism of superconductivity. To understand this phenomenon, direct measurements of glassy charge order are needed.

Background problem in resonant soft x-ray scattering (RSXS)



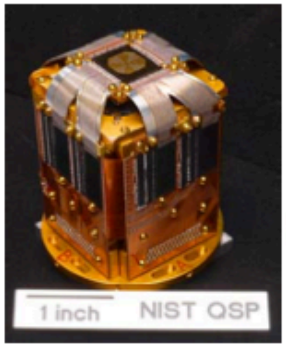
The most direct way to measure charge order is RSXS, which has previously shown that that valence band order exists in both 214 cuprates, such as $La_{2-x}Ba_xCuO_4$ and 123 materials such as $YBa_2Cu_3O_{7-\delta}$.

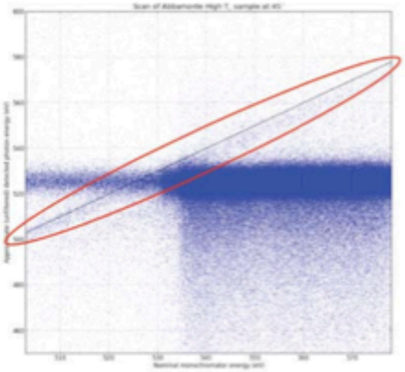
Unfortunately, inelastic background problems prevent detection/study of short-ranged order.

TES array detectors with high-resolution *will eliminate this background.*

The new TES array detector at IEX-CDT at APS is of the same type used to detect gravity waves at BICEP2.

This array has **1 eV intrinsic energy resolution**, eliminating background and enabling—for the first time—studies of short-ranged order with RSXS.

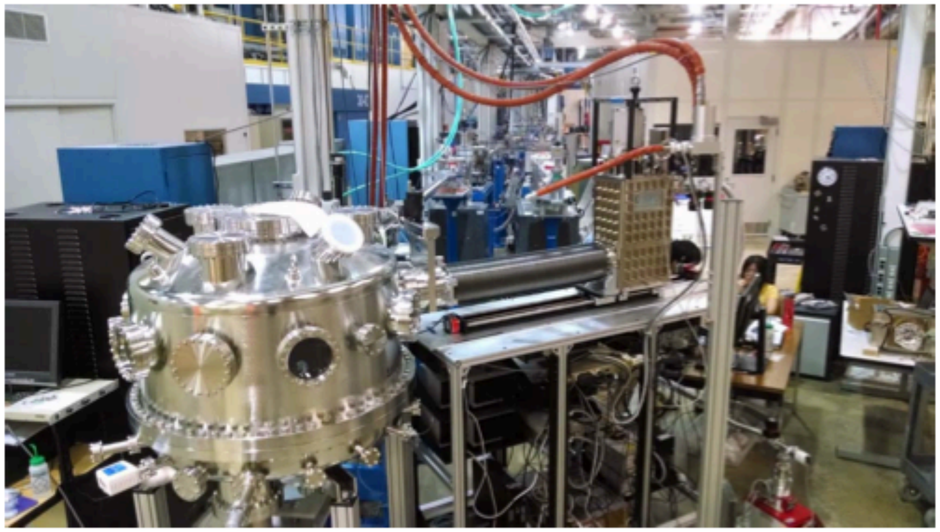




References:

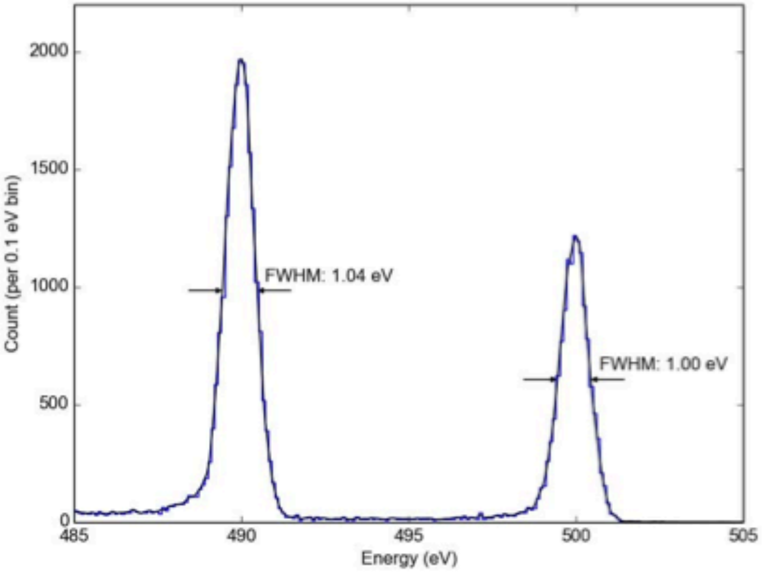
- Hanaguri, Nature **430**, 1001 (2004)
- Abbamonte, Nature Phys. **1**, 155 (2005)
- Ghiringelli, Science **337**, 821 (2012)

Update, Sept. 2014



Resonant scattering endstation
IEX-CDT, Sector 29
Advanced Photon Source

Successful TES test, Aug. 2014



U.S. DEPARTMENT OF ENERGY | Office of Science

ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

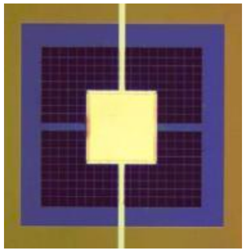
NIST

Argonne NATIONAL LABORATORY

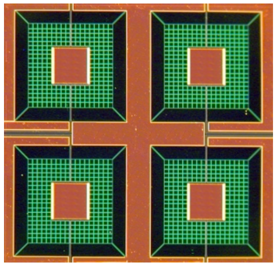
Courtesy of Kent Irwin

TES spectrometer Moore's Law: ~2 years doubling

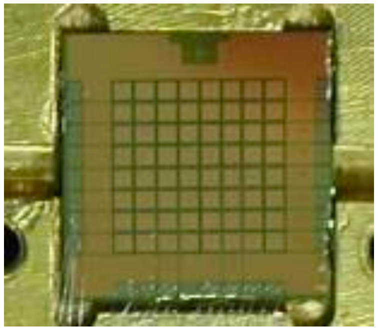
1 pixel
1996

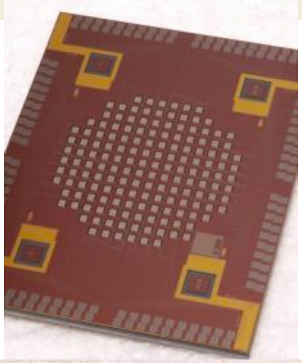


4 pixel
2000

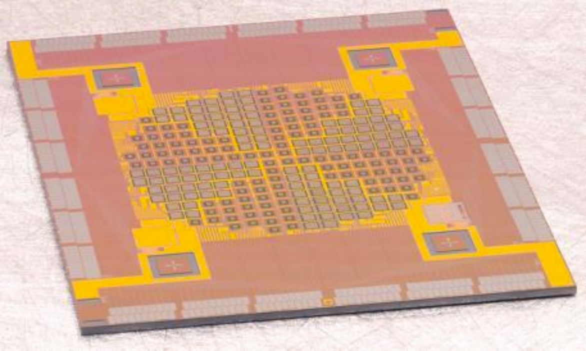


24 pixel
2004

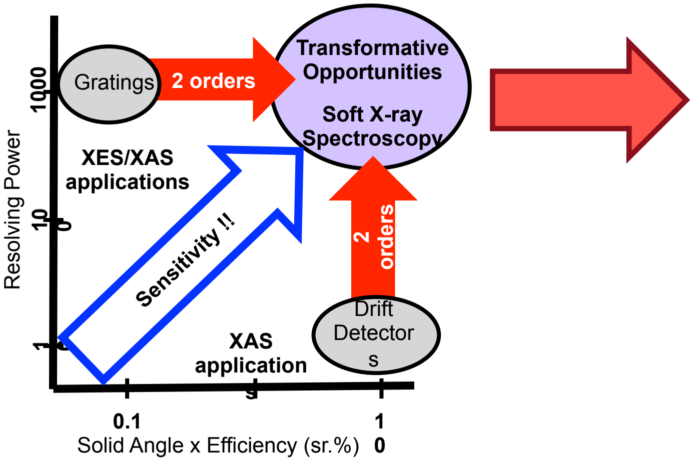




45 pixel
2008



240 pixel
2014



Long-term program will double solid angle & count rate every ~ two years

Challenges

- Detector comprises
  - Sensors
    - Material / technology challenges
    - Design / technology challenges
  - Electronics (Front/back end)
    - Functionalities, power, IGR challenges
- Detector produces
  - More and more data
    - Links and data reduction challenges
- Methods
  - Setups and analysis challenges
    - Convergence

Thanks !

Other contributors

SLAC detector group
SLAC DAQ, controls and data group
LCLS instrument scientists
SSRL beamline scientists and support
Etc. etc.